OMNIS Software 4.2.0

Product manual

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Technical Communication
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1 Overview

1.1 OMNIS system – Information

OMNIS, the new modular platform for wet-chemistry laboratory analysis

Depending on requirements, OMNIS can be extended from a simple stand-alone titrator to a fully automated robot that can process a maximum of 175 samples while performing up to four analyses simultaneously.

In accordance with the pick-and-place principle, the OMNIS sample robot continuously serves up to four workstations at which up to four analyses can be carried out in parallel. If OMNIS finds free capacity at a workstation, it will be used automatically for the next analysis.

Through its use of a patented Liquid Adapter, OMNIS makes reagent replacement simpler than ever before. When the Liquid Adapter snaps in, OMNIS extracts the information regarding the contents of the bottle that is saved to an RFID chip and stores it in the software. With the automatic identification and checking of the reagents, OMNIS closes the last gap in the traceability of the entire analysis.

OMNIS can be operated intuitively. Configuration of work systems could not be easier: the respective components are simply moved into the work area with drag and drop. The graphic method editor also functions in

accordance with the same principle: Users select one command after another with drag and drop and thus assemble "their" methods.

OMNIS assembles the results for all of the parameters of interest across all methods and links the results to the respective sample.

Technical features at a glance

1. Operation via PC (or by touch screen).
2. OMNIS system can be operated from any location.
3. High-precision dosing.
4. Fully automated analysis, individually extendable up to 175 samples.
5. Space-optimized instrument design for minimum laboratory bench requirements.
6. Simple presentation of the OMNIS system status.
7. Quick and safe reagent replacement via Liquid Adapter.

1.2 OMNIS Software – About the documentation

Read through this documentation carefully before putting the software into operation.

The documentation contains important information and warnings that must be followed for safe operation of the software.

Symbols and conventions

The following icons and formatting may appear in this documentation:

(**1**)	**Reference to the position number** The number corresponds to the position number in the figure within an instruction step.
(*(see figure "caption")*/1)	**Reference to the figure and position number** The link refers to the caption and the number to the position number in a figure outside of the instruction step.
1	**Instruction step** These steps are carried out in sequence.
Method	Designations for names of parameters, menu items, tabs and dialog windows in the software.
Processes ▶ Operating procedures	**Menu path** Display of paths within the software. The last part shows the target or the level at which the action is performed or where the information can be found.

[Next]	**Button** or **key**

1.3 Software help – Welcome – OMNIS Help

The OMNIS Software contains a comprehensive Help feature that can be accessed from the software and that is displayed in the default browser window under the name **OMNIS Help**. Information on all the functions of the OMNIS Software are available there.

All the OMNIS Software functions are described in the Help feature. The functionality in the software that a user can see or use depends on their individual rights. Additional information on the rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

If you require a described functionality and you do not have the corresponding right, then please contact your internal IT administrator.

If data permission filtering is activated, then it depends on the assigned data permissions which data in the software is visible or usable for a user. Additional information: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

Contact your data permissions manager if the assignment of the data permissions needs to be adjusted.

Accessing the OMNIS Help

There are several ways how to access the software help (**OMNIS Help**):

- Click on the **OMNIS Help** button in the title bar under • • •.
- Press the **[F1]** key.
- Clicking on **?** in various areas or windows results in the context-sensitive display of the Help feature for this element.

Content of the OMNIS Help

The Help function is automatically installed in German, English and Chinese when the OMNIS Software is installed. The following documents are also available:

- The user interface in additional languages: *Installing language packs*.
- The software help in additional languages: *(see "Importing software help", chapter 3.1, page 10)*.

Information packs on OMNIS hardware components can also be loaded manually into the software help (*(see "Importing software help", chapter 3.1, page 10)*). The following documentation is available:

- Product manuals (link is visible only if manuals have already been loaded):
- Sensor leaflets (link is visible only if leaflets have already been loaded): *Sensor leaflet* (Metrohm Knowledge Base)

Searching and filtering

In the **OMNIS Help**, you can search through the entire content for the required information using a full-text search. The filters (left-hand part of window) can also be used to display specific content. For an overview on navigation: *(see "Software help – Overview – OMNIS Help", chapter 1.4, page 5)*

Further information on the OMNIS Software

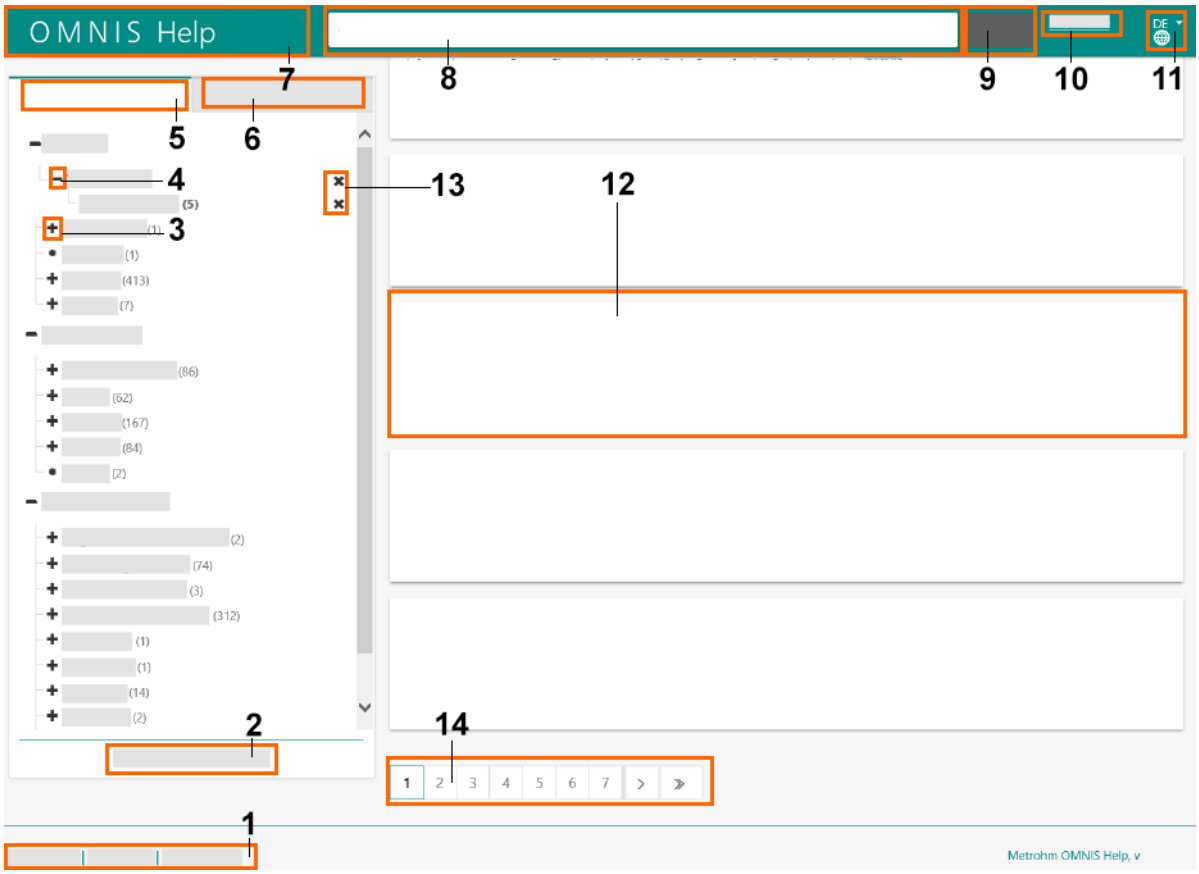
In addition to the **OMNIS Help**, which is installed locally on the computer, all information on software functions and OMNIS hardware components is available online in the Metrohm Knowledge Base *https://guide.metrohm.com/*

See also

Importing software help (chapter 3.1, page 10)

Software help – Overview – OMNIS Help (chapter 1.4, page 5)

1.4 Software help – Overview – OMNIS Help



1 Additional links
Link to Metrohm AG website and information on imprint and legal matters.

2 Resetting filters
All selected filters are reset.

3 Expanding a filter
Click on the filter criteria to activate filtration. The structure can be expanded with +.

4 Collapsing a filter
Click on the filter criteria to activate filtration. The structure can be collapsed with —.

5 Filter
Possibility of filtering the search results.

If the search delivers many hits, the hit list can be filtered. The number of hits is displayed for each filter criterion.

6 Table of contents
Display of the table of contents for the product manuals to which a topic belongs (only selectable on topic-level).

7 **Welcome start page**
Link back to the start page.

8 **Input field**
Input of a search term.

OR: Display of contents in which one or the other character string is contained.

[*]: Display of all available contents.

9 **Search**
The entered search term is searched for in all contents by clicking on this icon or with **[Enter]**.

10 **All contents**
Link for displaying all published contents.

11 **Language settings**
Selection of the desired language.

12 **Search result**
Search result with short information on the content of the topic. The number of contents found with corresponding short information is displayed under **Search results**.

13 **Unselecting a filter**
Unselect individual filter criteria.

14 **Scrolling search results**
Flip through the search results if the number of search hits found exceeds one screen page.

See also

Software help – Welcome – OMNIS Help (chapter 1.3, page 3)

2 Safety

2.1 Intended use

Metrohm products are used for the analysis and handling of chemicals.

Usage therefore requires the user to have basic knowledge and experience in handling chemicals. Knowledge regarding the application of fire prevention measures prescribed for laboratories is also mandatory.

Adherence to this technical documentation and compliance with the maintenance specifications make up an important part of intended use.

Any utilization in excess of, or deviating from, the intended use is regarded as misuse.

Specifications regarding the operating values and limit values of individual products are contained in the "Technical specifications" section, if relevant.

Exceeding and/or not observing the mentioned limit values during operation puts people and components at risk. The manufacturer assumes no liability for damage due to non-observance of these limit values.

The EU declaration of conformity loses its validity as soon as modifications are carried out on the products and/or the components.

See also

Instruments – Directory (chapter 5.12.2.2, page 854)

2.2 Responsibility of the operator

The operator must ensure that basic regulations on occupational safety and accident prevention in chemical laboratories are observed. The operator has the following responsibilities:

- Instruct personnel in the safe handling of the product.
- Train personnel in the use of the product according to the user documentation (e.g. install, operate, clean, eliminate faults).
- Train staff on basic occupational safety and accident prevention regulations.
- Provide personal protective equipment (e.g. protective glasses, gloves).
- Provide suitable tools and equipment to carry out the work safely.

The product may be used only when it is in perfect condition. The following measures are required to ensure the safe operation of the product:

- Check the condition of the product before use.
- Remedy defects and malfunctions immediately.

- Maintain and clean the product regularly.

2.3 Requirements for operating personnel

Only qualified personnel may operate the product. Qualified personnel are persons who meet the following requirements:

- Basic regulations on occupational safety and accident prevention for chemical laboratories are known and complied with.
- Knowledge of handling hazardous chemicals is present. Personnel have the ability to recognize and avoid potential dangers.
- Knowledge regarding the application of fire prevention measures for laboratories is available.
- Safety-relevant information is communicated and understood. The personnel can operate the product safely.
- The user documentation has been read and understood. The personnel operate the product according to the instructions in the user documentation.

2.4 Safety instructions

2.4.1 Danger from electrical potential

Contact with electrical potential can cause serious injuries or death. To avoid danger from electrical potential, observe the following:

- Operate the product only if it is in perfect condition. The housing must also be intact.
- Only use the product with the covers fitted. If covers are damaged or missing, disconnect the product from the energy supply and contact the regional Metrohm service representative.
- Protect live components (e.g. power supply unit, power cord, connection sockets) against moisture.
- Always have maintenance work and repairs on electrical components carried out by a regional Metrohm service representative.
- Disconnect the product from the energy supply immediately if at least one of the following cases occurs:
  - The housing is damaged or open.
  - Live parts are damaged.
  - Moisture penetrates.

2.4.2 Dangers due to automated motion sequences

Product parts that move automatically (e.g. robot arm) can cause injuries due to crushing or clamping. To avoid the risk of injury, observe the following:

- Do not reach into the working area of the products during the work process.

- Install and use the protective devices enclosed with the product during the work process.
- Do not bypass the installed protective devices.

3 After installation

3.1 Importing software help

The default languages for the **OMNIS Help** are installed automatically at the time of the installation of the OMNIS Software. Additional languages, product manuals and sensor leaflets (**OMNIS Help Add-Ons**) can be manually imported later.

Prerequisite:

- The Windows user currently logged on has the local administrator rights.
- The latest version of a browser is installed.
- The OMNIS Software is installed.
- The language packs are installed according to the instructions: *Installing a language pack*.

1 Opening a browser

- Open a current browser.
- Enter the link *https://www.metrohm.com/en/service/software-center/omnis-help-packages.html* in the address line and confirm the address by clicking **[Enter]**.

2 Downloading a ZIP file

- Select the required software help (**OMNIS Help Add-Ons**) and save the corresponding ZIP file to your computer (e.g. to the desktop).

3 Opening Explorer

- Open the local Explorer.
- Open the **...\Metrohm\OMNIS\TopicPilot\context\importer\hotfolder\default** folder in the installation pathway of the OMNIS Software.

4 Importing a ZIP file

- Copy the downloaded ZIP file into this folder.

The **OMNIS Help** automatically loads all the files and then deletes the corresponding ZIP file from this folder. Restarting the OMNIS Software is not necessary.

Multiple ZIP files can also be copied into the folder.
The installation process takes a few minutes. The installation is not complete until there are no files present anymore in the **...\Metrohm\OMNIS\TopicPilot\context\importer\hot-folder\default** folder.

See also

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Software help – Overview – OMNIS Help (chapter 1.4, page 5)

Software help – Welcome – OMNIS Help (chapter 1.3, page 3)

3.2 Importing the templates

Metrohm provides templates for operating procedures and methods to make your work easier. Proceed as follows to import these templates into the OMNIS Software:

1 Downloading the templates

- The templates can be found under the following link: *Operating procedure – Templates for titration* / *Operating procedures/methods – Templates for TitrIC flex*
- If your computer, on which the OMNIS Software is installed, has no Internet access, you can search for the templates on another computer with Internet access under *guide.metrohm.com* using the keyword **Template** and download them from there.
- Click on **[Download]** in the opened topic.
- Save the ZIP file.

2 Unpacking the templates

- Unpack the ZIP file using a suitable ZIP tool (e.g. WinZip).

The unpacked folder contains the operating procedures and methods as OPRO files.

3 Importing the templates

- Click on to open the **Import data** window in **Processes** ▶ **Operating procedures** or in **Processes** ▶ **Methods**.
- Open the folder with the unpacked templates, select the desired OMNIS process files and click on **[Open]**.

The operating procedures and methods are imported into the OMNIS Software.

If the operating procedure or method contains work systems, then these are also imported.

The templates need to be adapted to your system. Important information and help can be found in the descriptions of the templates: *Operating procedure – Templates for titration* / *Operating procedures/methods – Templates for TitrIC flex*

See also

Operating procedure – Definition (chapter 5.11.1, page 379)

4 Start-up

4.1 OMNIS Client/Server system – Definition

The OMNIS Software can be operated as an **OMNIS Client/Server system**. The **OMNIS Client/Server system** is used to store generated data centrally on the OMNIS Server and make it available to all OMNIS Clients. This enables data exchange between multiple OMNIS Clients and supports central data backup. The **OMNIS Client/Server system** must be selected at the time of initial installation. No subsequent change to an **OMNIS Client/Server system** is then possible.

Additional OMNIS Clients can be added to the **OMNIS Client/Server system**. This makes the **OMNIS Client/Server system** scalable.

To carry out service activities the operation mode on the OMNIS Server and the individual OMNIS Clients can be changed. The operation mode of the OMNIS Client must correspond to the operation mode on the OMNIS Server. Additional information on the operation mode: *(see "Operation mode – Definition", chapter 6.1.7, page 1233)*

Data that is synchronized with the OMNIS Server:

- Subsamples with published operating procedures
- Subsamples with unpublished operating procedures, depending on the status
- Samples depending on their subsamples
- Server search queries
- Published sample profiles
- Published operating procedures and methods and the associated methods model hierarchies and slope/y-intercept corrections
- Published work systems
- All Audit Trail entries
- All data and settings from the **User management** work area
- All settings from the **Advanced settings** subsection
- Data permissions

All the OMNIS Client/Server system functions are described in the Help feature. The functionality in the software that a user can see or use depends on their individual user rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

The following rules apply in the OMNIS Client/Server system:

- Each OMNIS Client works with the local database **(Microsoft SQL Server Express, 10 GB)** and synchronizes with the OMNIS Server within the **OMNIS Client/Server system**. The OMNIS Server works with an external database on which generated data is centrally stored. This data is available to all connected OMNIS Clients. In offline mode, the OMNIS Client can access solely the locally available data. All created and changed data is saved to the local database. Automatic synchronization takes place as soon as the OMNIS Client is connected to the OMNIS Server again. The option to work in offline mode is provided only in exceptional situations (e.g. if the OMNIS Server is temporarily unavailable for technical reasons).
- If several users edit the same data at the same time, the changes of the user whose OMNIS Client synchronizes with the OMNIS Server first are applied. Other users are informed that their changes have not been synchronized and that the last change may need to be repeated.
- If a user makes manual changes to a subsample that is being used at the same time in a determination on another OMNIS Client, then those changes will be applied from the determination. The results of a determination overwrite the manual changes and the other user is informed that his or her changes have not been synchronized and that the last change may need to be repeated.
- The functions and the user interface of the **OMNIS Client/Server system** are visible and usable for a user only if the **OMNIS Client/Server system** was selected at the time of the installation of the OMNIS Software.

- Software licenses of the **OMNIS Client/Server system** are managed centrally (central licensing) and temporarily conferred by the OMNIS Server to all connected OMNIS Clients automatically. Separate software licenses are required for the **OMNIS Client/Server system**. Additional information on the respective license version can be obtained at *http://www.metrohm.com* or from your regional Metrohm representative. The software licenses are enabled on the first OMNIS Client as standard. Subsequent activation of additional software licenses can be accomplished from any connected OMNIS Client. In the event of a loss of connection between the OMNIS Server and the OMNIS Client, the borrowed software licenses are valid for 48 hours. This means that the OMNIS Client can be used without interruption during this period and instruments that have already been reserved also retain their functionality. The activated and borrowed software licenses can be accessed on the *license container*.
- The connection status of the OMNIS Server is indicated by the icon in the top right corner of the OMNIS Software title bar.
- Communication between the OMNIS Clients and the OMNIS Server is secured by the use of certificates. During initial installation, it is possible to determine whether self-signed or customer-specific certificates are used. Certificates can be changed subsequently via the Windows command prompt *(Manage certificates)*.

In the OMNIS Client/Server system, the following rules apply for the Samples work area:

- Samples and subsamples from an OMNIS Client are automatically loaded onto the OMNIS Server when the corresponding sample list is saved if the following conditions are met:
  - All subsamples associated with the sample are saved and have no local changes.
  - All subsamples associated with the sample use a published operating procedure or they have already been analyzed. Subsamples that use a published operating procedure are always loaded onto the OMNIS Server. Subsamples that use an unpublished operating procedure are only loaded onto the OMNIS Server if they are in the **Completed** or **Edited** status.
- Samples and subsamples on the OMNIS Server can be searched in **Server search queries** using filter criteria. The results of a server search query can be selected and transferred to a new sample list. This downloads the samples and subsamples and they can be used locally on the OMNIS Client.

- A sample can be downloaded from the OMNIS Server only if the following conditions are met:
  - The subsamples associated with the sample have not been deleted from the OMNIS Server.
  - All subsamples associated with the sample are in the status **Ready**, **Completed**, **Canceled** or **Edited**.
- Metrohm recommends deleting samples and subsamples only when the connection to the OMNIS Server is available in order to preclude any synchronization errors.
- A sample is always downloaded with all associated subsamples. Downloading multiple samples results in their being treated as a package. If there is a problem with a subsample during download, then none of the selected samples will be downloaded and no new sample list will be created.
- When a sample is downloaded, associated published operating procedures, published methods, work systems, models, model hierarchies, and slope/y-intercept corrections are also downloaded so that they can be executed immediately after downloading.
- Downloaded samples and subsamples are synchronized on the OMNIS Client each time the respective sample list is updated or opened, thus showing the current changes (e.g. due to determinations).
- Sample profiles containing only published operating procedures can be published.
- Published sample profiles are available to all connected OMNIS Clients. They must first be downloaded in order to be subsequently used for a determination. Downloaded sample profiles can be adapted and saved with the changes on the local OMNIS Client. To save the changes of a downloaded sample profile on the OMNIS Server, the sample profile must be republished.
- The associated sample data (operating procedures, methods, work systems, models, model hierarchies, and slope/y-intercept corrections) is also downloaded when a published sample profile is downloaded.
- The server sample profile can be deleted from the OMNIS Server. The deleted sample profile is retained locally on the connected OMNIS Clients that downloaded the server sample profile before it was deleted.
- The associated sample data (operating procedures, methods, work systems, models, model hierarchies and slope/y-intercept corrections) is not deleted when a published sample profile is deleted.
- When importing a published sample profile into an **OMNIS Stand-Alone**, the respective status (published, contains withdrawn or deleted objects) is not imported.
- When exporting a published sample profile, the respective status is exported.

- When duplicating a published sample profile, the respective status is not duplicated because new objects are created in the OMNIS Software when duplicating.
- The current status of a server sample profile is indicated by a corresponding icon.
- The server sample profiles can be filtered by name.

In the OMNIS Client/Server system, the following rules apply for the Processes work area:

- The published operating procedures and methods are available for all connected OMNIS Clients and are protected against changes.
- When publishing an operating procedure, the associated methods, work systems, models, model hierarchies, and slope/y-intercept corrections, solution conditions, and sensor conditions are also published. When publishing a method, the associated work systems, models, model hierarchies, slope/y-intercept corrections, solution conditions, and sensor conditions are also published. When publishing an operating procedure or method that contains the **ADD TO SAMPLE LIST** command, the referenced operating procedures and associated methods are also published if they have not already been published. The sample data is applied from the referenced sample profile.
- The associated methods, work systems, models, model hierarchies, slope/y-intercept corrections, solution conditions, and sensor conditions are also downloaded when a published operating procedure is downloaded. The associated work systems, models, model hierarchies, slope/y-intercept corrections, solution conditions, and sensor conditions are also downloaded when a published method is downloaded. When downloading an operating procedure or method that contains the **ADD TO SAMPLE LIST** command, the referenced operating procedures and associated methods are downloaded only if they are the same as the published server operating procedures and server methods.
- In order to limit the use of a published operating procedure or method by other users, it can be withdrawn or deleted.
- The associated methods, work systems, models, model hierarchies, and slope/y-intercept corrections are not themselves withdrawn when a published operating procedure is withdrawn. When withdrawing a published method, the associated work systems, models, model hierarchies and slope/y-intercept corrections are not themselves withdrawn.

- Only a withdrawn server operating procedure or server method can be deleted. The deleted operating procedure or method is retained locally in the status **withdrawn** on connected OMNIS Clients which downloaded the server operating procedure or server method before it was deleted.
- The current status of a server operating procedure and server method is indicated by a corresponding icon.
- Only a published operating procedure or method can be signed. To be able to sign a published operating procedure, all the associated methods must first be signed.
- The signature can be added to a published operating procedure or method in **Processes** ▶ **Operating procedures** or **Methods**.
- If an operating procedure or method that has already been signed is to be published, then the signature must first be deleted and then added again after publication.
- Solution conditions and sensor conditions can be defined for the functional unit of a command only before the publication of the method or the operating procedure.
- After a published operating procedure has been downloaded that contains a method with a command with defined solution conditions or sensor conditions, that method and that command will be indicated in the operating procedures editor with . After a published method has been downloaded that contains a command with defined solution conditions or sensor conditions, the command will be indicated in the method editor with .
- When importing a signed, published or withdrawn operating procedure or method into an **OMNIS Stand-Alone**, only existing signatures are imported. The respective status (published, withdrawn, unusable) is not imported.
  If the **Import with work system** check box is enabled at the time of the import, then the work system is imported with the defined solution conditions and sensor conditions. The defined solution conditions and sensor conditions are also imported if the work system used in the imported operating procedure or method is already available, even though the **Import with work system** check box is disabled.
- When exporting a signed, published or withdrawn operating procedure or method, the respective status and any signatures, models, model hierarchies, slope/y-intercept corrections, solution conditions, and sensor conditions are also exported.

- When duplicating a signed, published or withdrawn operating procedure or method, the respective status and any signatures will not be duplicated because new objects are created in the OMNIS Software during duplication.
  The new operating procedure or method will contain the same operating procedures, models, model hierarchies, slope/y-intercept corrections, solution conditions and sensor conditions as the original operating procedure or method.
- Solution conditions and sensor conditions are stored in the method and defined for the functional unit of the work system. If the conditions are also to be taken into account in the execution of a downloaded method or operating procedure, then precisely the same functional units must be used as in the published server method or server operating procedure. If the original work system is replaced by a work system of its own, then the defined solution conditions and sensor conditions are lost.
- Tags can be created, added and removed in the server operating procedures and server methods.
- The server operating procedures and server methods can be filtered by names and tags.

In the OMNIS Client/Server system, the following rules apply for the Audit Trail work area:

- All Audit Trail entries of the connected OMNIS Clients are stored centrally on the OMNIS Server. All entries can be viewed in the Audit Trail on all connected OMNIS Clients.
- If the connection to the OMNIS Server is interrupted, only the local Audit Trail entries are displayed. Therefore, it must be noted that the entries may be incomplete in case of an interrupted connection.

In the OMNIS Client/Server system, the following rules apply for the User management work area:

- An activated user management (**User management (OMNIS)** or **User management with Active Directory integration**) is a prerequisite for the use of the **OMNIS Client/Server system**. The OMNIS Software does not need to be restarted after successful setup of user management. The administrator performing the setup can log in directly to the OMNIS Software in the last dialog of the setup.
- The settings made in user management are valid in the **OMNIS Client/Server system** for all connected OMNIS Clients (central user management). The users of all OMNIS Clients are created, edited or deactivated centrally in the **OMNIS Client/Server system**.
- The user rights as well as the security settings are managed centrally and are valid in the **OMNIS Client/Server system** for all connected OMNIS Clients.

- Metrohm recommends configuring settings in the **User management** work area only when the connection to the OMNIS Server is available, in order to preclude any synchronization errors.

In the OMNIS Client/Server system, the following rules apply for the Settings work area:

- The system language, user management and conformity functions are managed centrally and are valid in the **OMNIS Client/Server system** for all connected OMNIS Clients (central management of the **Advanced settings**).
- **General settings** (dialog language, emergency stop function, Include preliminary run test, print settings and notification settings) apply only for 1 OMNIS Client.
- Metrohm recommends making changes in the **Settings** work area only when the connection to the OMNIS Server is available, in order to preclude any synchronization errors.

The requirements for the OMNIS system can be found under: *System requirements – Technical White Paper*.

See also

Activating the software license (chapter 4.2.1, page 29)

Audit Trail – Directory (chapter 5.14.5, page 1177)

Data permissions – Definition (chapter 4.5.9, page 105)

Database – Definition (chapter 4.6, page 117)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

Managing an OMNIS Client (chapter 4.1.2, page 22)

Methods – Subsection (chapter 5.11.3.1, page 414)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Processes – Actions (chapter 5.11, page 378)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Publishing the sample profile (chapter 5.10.5.5, page 267)

Sample profiles – Status (chapter 5.10.5.6, page 269)

Sample profiles – Subsection (chapter 5.10.5.1, page 259)

Samples – Actions (chapter 5.10, page 208)

Server method – Definition (chapter 5.11.4, page 425)

Server methods – Subsection (chapter 5.11.4.1, page 426)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Server operating procedures – Subsection (chapter 5.11.2.1, page 412)

Server sample profile – Definition (chapter 5.10.6, page 270)

Server sample profiles – Subsection (chapter 5.10.6.1, page 271)

Settings – Actions (chapter 5.15, page 1197)

User rights – Directory (chapter 4.5.7.4, page 89)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

4.1.1 OMNIS Server – Status

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

In the **OMNIS Client/Server system**, the connection status of the OMNIS Server is displayed as follows:

Display in the title bar

	OMNIS Server connected The OMNIS Software is connected to the OMNIS Server.
	Connecting to the OMNIS Server The OMNIS Software tries to reconnect to the OMNIS Server every 30 seconds. Meanwhile, the status is displayed in orange. Each attempt lasts 10 seconds and attempts are continued until the connection to the OMNIS Server is restored. Data that is current or recently changed may not have been synchronized. The data is synchronized as soon as the connection has been restored.
	OMNIS Server not connected The attempts to reconnect have failed. The connection between the OMNIS Software and the OMNIS Server is interrupted. Data that is current or recently changed cannot be synchronized. The data is synchronized as soon as the connection has been restored.

OMNIS Server not compatible

The OMNIS Software cannot connect to the OMNIS Server. The version of the OMNIS Client used is not compatible with the OMNIS Server. Data that is current or recently changed cannot be synchronized. The data is synchronized after this version conflict has been solved.

Differently configured operation modes

The OMNIS Software cannot connect to the OMNIS Server. The OMNIS Client and the OMNIS Server are in non-compatible operation modes due to an incorrect configuration. The offline mode prevents a data loss. The connection to the OMNIS Server is re-established once the OMNIS Client and the OMNIS Server are in the same operation mode. To do this, problems with the configuration may have to be rectified by the internal IT administrator.

The operation mode of the OMNIS Client can be changed in the **OMNIS Database Administration** program or in the OMNIS Software under **Settings ▶ Database settings**.

See also

Changing the operation mode (chapter 6.1.8, page 1233)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Database Administration – Actions (chapter 6.1, page 1207)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Operation mode – Definition (chapter 6.1.7, page 1233)

4.1.2 Managing an OMNIS Client

- After the initial installation of the OMNIS Software as **OMNIS Client/Server system**, further OMNIS Clients can be added to the OMNIS system: *Adding an OMNIS Client*
- If for example the hardware is damaged, then existing OMNIS Clients can be replaced: *Replacing an OMNIS Client*
- OMNIS Clients can be deleted from the OMNIS system via the Windows command prompt. OMNIS Clients can be deleted only on the computer on which the OMNIS Server is installed: *Deleting an OMNIS Client*

It is not necessary to license the software or activate the user management when adding further OMNIS Clients or when replacing existing OMNIS Clients. The activation of necessary software licenses and the user

management is only carried out on the 1st OMNIS Client. The necessary software licenses are automatically allocated to each OMNIS Client by the OMNIS Server.

OMNIS Clients can only be managed in the Main operation mode. Further information on the operation modes: *Definition operation mode*

Adding an OMNIS Client

Prerequisite:

- The 1st OMNIS Client was added to the **OMNIS Client/Server system**.
- The OMNIS Client has been started in the Main operation mode.
- A connection to the OMNIS Server and to the Metrohm license server is available.
- An Internet connection is available.
- The customer number (format: 123-456789) is available.
- The Windows user currently logged on has the local administrator rights.

1 Starting the OMNIS Software

- Start the OMNIS Software.

The wizard for activating the OMNIS Client appears.

2 Selecting the activation mode

- Select the **Add new OMNIS Client** option.
- Start the activation of a new OMNIS Client by clicking on **[Next step]**.

3 Entering the customer number

- Enter the correct **Customer number**.

The customer number entered is verified.

4 Entering the name of the OMNIS Client

- Enter a unique name for the OMNIS Client and click on **[Next step]**.

The chosen name can only be used once in the entire **OMNIS Client/Server system**. A maximum of 24 characters can be entered. The following special characters must not be used: / \ ? * % ; ' " : | [ ] + = , < > @

After the name of the OMNIS Client has been verified successfully, it is added to the **OMNIS Client/Server system**. After that, the user of the OMNIS Client can log into the OMNIS Software.

If an invalid ticket number was entered during the offline licensing, an additional field appears after the verification of the customer number where the correct ticket number can be entered again.

Adding a new OMNIS Client is possible if the computer with the OMNIS Software has direct Internet access. If the computer with the OMNIS Software does not have direct Internet access, another computer with Internet access has to be used. It must be possible to exchange data between both computers, e.g. via a USB flash drive. Follow the instructions of the wizard for adding a new OMNIS Client in the offline mode.

Replacing an OMNIS Client

Prerequisite:

- At least one OMNIS Client is available in the **OMNIS Client/Server system**.
- The OMNIS Client has been started in the Main operation mode.
- A connection to the Metrohm license server is available.
- An Internet connection is available.
- The customer number (format: 123-456789) is available.
- The Windows user currently logged on has the local administrator rights.

1 Starting the OMNIS Software

- Start the OMNIS Software.

The wizard for activating the OMNIS Client appears.

2 Selecting the activation mode

- Select the **Replace existing OMNIS Client** option.
- Start the replacement of an existing OMNIS Client by clicking on **[Next step]**.

3 Entering the customer number

- Enter the correct **Customer number**.

The customer number entered is verified.

4 Loading OMNIS Clients

- Load all the currently existing OMNIS Clients in the **OMNIS Client/Server system** by clicking on **[Load OMNIS Clients]**.

The names of all OMNIS Clients that are assigned to the previously entered customer number are displayed in the selection list at the bottom of the dialog.

5 Selecting the name of the OMNIS Client

- Select the OMNIS Client that is to be replaced from the selection list of the existing OMNIS Clients and click on **[Next step]**.

The selected OMNIS Client is replaced. After that, the user can log into the OMNIS Software on the new OMNIS Client.

If an invalid ticket number was entered during the offline licensing, an additional field appears after the verification of the customer number where the correct ticket number can be entered again.

Replacing an existing OMNIS Client is possible if the computer with the OMNIS Software has direct Internet access. If the computer with the OMNIS Software does not have direct Internet access, another computer with Internet access has to be used. It must be possible to exchange data between both computers, e.g. via a USB flash drive. Follow the instructions of the wizard for the replacement of an existing OMNIS Client in the offline mode.

Deleting an OMNIS Client

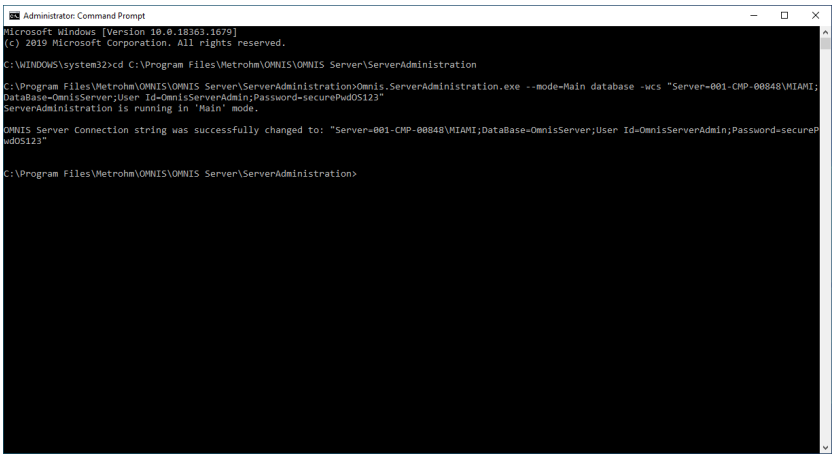
Prerequisite:

- The **OMNIS Client/Server system** is installed.
- The OMNIS Client to be deleted is closed and no process associated with it is being carried out (e.g. deleting, archiving, removing).
- The OMNIS Server has been started in the Main operation mode.
- The Windows user currently logged on has the local administrator rights.

1 Switching to the OMNIS Server in a command prompt

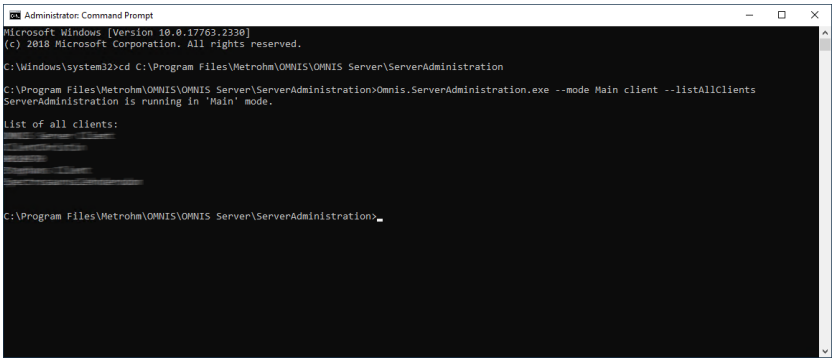
- Open the Windows start menu.
- Search for the Windows command prompt. Open the context menu by right-clicking and select **Run as administrator**.

- Enter the text **cd** (change directory) followed by a space and then enter the installation pathway of the OMNIS Server (**C:\Program Files\Metrohm\OMNIS\OMNIS Server\ServerAdministration** by default).
- Confirm the entry with **[Enter]**.



2 Listing the names of the OMNIS Clients

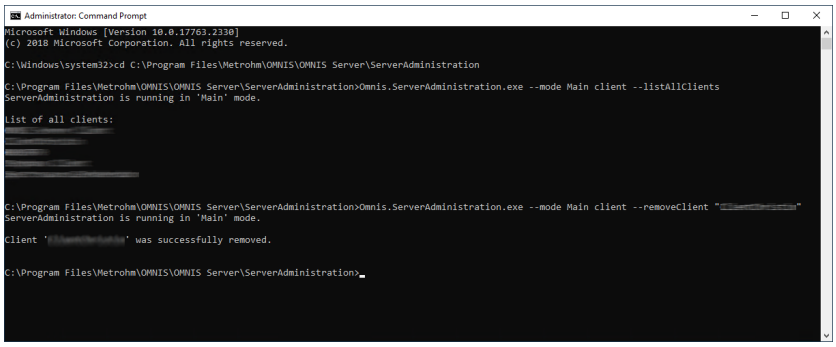
- Enter the following text line in the command prompt: Omnis.ServerAdministration.exe --mode Main client --listAllClients
- Confirm the entry with **[Enter]**.



The names of all OMNIS Clients that have been added to the **OMNIS Client/Server system** are listed.

3 Deleting an OMNIS Client

- Enter the following text line in the command prompt: Omnis.ServerAdministration.exe --mode Main client --removeClient {"NAME OF CLIENT"}



The 1st OMNIS Client must not be deleted.

The OMNIS Client is deleted.

4 Updating and sending the OMNIS environment information

- Send the OMNIS environment information by following these instructions: *Sending the OMNIS environment information*

See also

Activating the software license (chapter 4.2.1, page 29)

Changing the operation mode (chapter 6.1.8, page 1233)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operation mode – Definition (chapter 6.1.7, page 1233)

User rights – Directory (chapter 4.5.7.4, page 89)

4.1.3 Offline mode – Definition

An offline mode is available in the **OMNIS Client/Server system** to prevent data loss when the connection to the OMNIS Server is interrupted. Offline mode activates automatically if the connection between the OMNIS Client and the OMNIS Server is interrupted.

In offline mode, the OMNIS Client can access solely the locally available data. This includes the following data:

- Own equipment such as sensors, reserved devices, solutions, etc.
- All objects in the OMNIS software that were either created locally or downloaded from the OMNIS Server before the connection was interrupted (e.g. samples, subsamples, methods, operating procedures or sample profiles).
- The user management with the settings before the connection was interrupted.

- All Audit Trail entries that were created on the respective client after the loss of connection.

The following functions are not available in offline mode:

- Access to all objects on the OMNIS Server (e.g. samples and subsamples on the OMNIS Server, published sample profiles, server operating procedures, server methods or published work systems).
- Downloading of samples and subsamples from the OMNIS Server.
- Uploading the locally created samples and subsamples to the OMNIS Server.
- Publishing sample profiles, methods, operating procedures and working systems.
- Synchronization of changes made by other OMNIS Clients in the **OMNIS Client/Server system**.
- Synchronization of local changes under **Advanced settings**.
- Creation of new data permissions.

In offline mode, all changes are saved only in the local database. Automatic synchronization takes place as soon as the OMNIS Client is connected to the OMNIS Server again.

The offline mode is provided only for exceptional situations (e.g. if the OMNIS Server is temporarily unavailable for technical reasons). After 48 hours in offline mode, the software licence becomes invalid and the OMNIS Client can be started again only if the server is accessible again and a software license for the OMNIS Client can be renewed. The local data is then automatically synchronized with the OMNIS Server.

See also

Activating the software license (chapter 4.2.1, page 29)

Data permissions – Definition (chapter 4.5.9, page 105)

Database – Definition (chapter 4.6, page 117)

Managing an OMNIS Client (chapter 4.1.2, page 22)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Server method – Definition (chapter 5.11.4, page 425)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Server sample profile – Definition (chapter 5.10.6, page 270)

User rights – Directory (chapter 4.5.7.4, page 89)

4.2 Licenses - Definition

- **Software license:** Software licenses can be used to enable individual software modules in the OMNIS Software. Additional information on activating software licenses: *Activating the software license*
- **Function license:** Function licenses can be used to enable individual instrument functions in the OMNIS Software. Additional information on activating function licenses: *Activating the function license*

Emergency licenses are made available to OMNIS users in emergencies. Additional information on the provision and use of emergency licenses:

If you have questions about licenses, contact your regional Metrohm representative.

4.2.1 Activating the software license

The OMNIS Software is modular in structure; the individual software modules can be licensed and activated individually. During initial installation of the OMNIS Software, an initial software license must be activated in order to use the OMNIS Software. Additional software licenses can be obtained and enabled later as required. If you have questions about software licenses, contact your regional Metrohm representative.

A software license that is already activated on the computer will also remain in effect in the event of an OMNIS Software version update. Contact your regional Metrohm representative if the computer in the OMNIS Stand-Alone needs to be replaced or exchanged.

In the **OMNIS Client/Server system**, the software licenses are centrally managed (central licensing) and allocated to all connected OMNIS Clients automatically by the OMNIS Server. The software licenses are enabled on the first OMNIS Client as standard. Subsequent activation of additional software licenses can be accomplished from any connected OMNIS Client. The activated and borrowed software licenses can be accessed on the *license container*. In the event of a loss of connection between the OMNIS Server and the OMNIS Client, the borrowed software licenses are valid for 48 hours.

Separate software licenses are required for the **OMNIS Client/Server system**. Additional information on the respective license version can be obtained at *http://www.metrohm.com* or from your regional Metrohm representative.

Additional information on the **OMNIS Client/Server system**: *OMNIS Client/Server system – Definition*

The activation of software licenses can only be carried out in the Main operation mode. Additional information on the operation modes: *Definition operation mode*

Enabling the initial software license

Prerequisite:

- The OMNIS Software is installed.
- The ticket number (format: 12345-12345-ABCDE-ABCDE-1X2Y3) is available.
- The customer number (format: 123-456789) is available.
- The Main operation mode was selected.

1 Starting the OMNIS Software

- Start the OMNIS Software.

A message appears.

2 Selecting the type of licensing

- Start online licensing or offline licensing by clicking on **[Continue]** or **[Continue offline]**.
- Follow the instructions of the licensing wizard.

- Online licensing is possible if the computer with the OMNIS Software has direct Internet access.
- Offline licensing must be selected if the computer with the OMNIS Software does not have direct Internet access and therefore another computer with Internet access has to be used. It must be possible to exchange data between both computers, e.g. via a USB flash drive.

3 Closing the licensing wizard

- Once the dialog **The license was successfully activated** appears, close the licensing wizard by clicking on **[Close]**. Click on **[Activate additional licenses]** and repeat step 2 if multiple software licenses need to be activated.

4 Activating the software license

Do not close the dialog during the licensing process. If the dialog is closed after entering the ticket number and starting the license activation process, then the licensing wizard will appear again the next time the OMNIS Software is started. Since a ticket number can be used only once, a new ticket number must be issued in this case or the **System Information Update** software license must be enabled.

- Activate the **System Information Update** software license.

Activating additional software licenses

Prerequisite:

- The OMNIS Software is installed.
- The ticket number (format: 12345-12345-ABCDE-ABCDE-1X2Y3) is available.
- The customer number (format: 123-456789) is available.
- The Main operation mode was selected.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory*

1 Starting the OMNIS Software

- Start the OMNIS Software.
- Under **Settings** ▶ **Software licenses**, click on **[Activate software licenses]** to start the licensing wizard.

A dialog is opened.

2 Selecting the type of licensing

- Start online licensing or offline licensing by clicking on **[Continue]** or **[Continue offline]**.
- Follow the instructions of the licensing wizard.

- Online licensing is possible if the computer with the OMNIS Software has direct Internet access.
- Offline licensing must be selected if the computer with the OMNIS Software does not have direct Internet access and therefore another computer with Internet access has to be used. It must be possible to exchange data between both computers, e.g. via a USB flash drive.

3 Closing the licensing wizard

- Once the dialog **The license was successfully activated** appears, close the licensing wizard by clicking on **[Close]**. Click on **[Activate additional licenses]** if multiple software licenses need to be activated.

See also

Changing the operation mode (chapter 6.1.8, page 1233)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operation mode – Definition (chapter 6.1.7, page 1233)

User rights – Directory (chapter 4.5.7.4, page 89)

4.2.2 Transferring a software license

In the **OMNIS Client/Server system**, the software licenses are centrally managed (central licensing) and allocated to all connected OMNIS Clients automatically by the OMNIS Server. The activated and borrowed software licenses can be accessed on the *license container*. In the event of a loss of connection between the OMNIS Server and the OMNIS Client, the borrowed software licenses are valid for 48 hours. Additional information on activating licenses: *Activating the software license*

Separate software licenses are required for the **OMNIS Client/Server system**. Additional information on the respective license version can be obtained at *http://www.metrohm.com* or from your regional Metrohm representative.

Additional information on the **OMNIS Client/Server system**: *OMNIS Client/Server system – Definition*

The transfer of software licenses can be carried out only in Main operation mode. Additional information on the operation modes: *Definition operation mode*

To transfer software licenses in the **OMNIS Client/Server system**, contact your regional Metrohm representative.

Online software license transfer

Prerequisite:

- The OMNIS Software is installed.
- An Internet connection is available.
- The Main operation mode has been selected.
- The user has the necessary rights. Additional information on the user rights: *Metrohm Knowledge Base*

1 Starting the OMNIS Software

- Start the OMNIS Software.

2 Opening the transfer wizard

- Open the transfer wizard by clicking on **[Transfer software licenses]** under **Software licenses** ► **Settings**.

A dialog is opened.

3 Selecting a transfer type

- Click on **[Continue]** to start the online transfer.

4 License removal

- Click on **[Continue]** to remove all licenses from this computer so that the licenses can be used on other computers.

All licenses are removed from the computer.

5 Saving a ticket number

- Click on **[Save ticket number]** to save the ticket number file and upload the file to the new computer. Follow the instructions for license activation: *Activating the software license*

6 Closing the transfer wizard

- As soon as the **Ticket number saved** dialog appears, click on **[Close]** to close the transfer wizard.

Offline software license transfer

Prerequisite:

- The OMNIS Software is installed.
- The Main operation mode has been selected.
- The user has the necessary rights. Additional information on the user rights: *Metrohm Knowledge Base*
- Contact your regional Metrohm representative to complete the license transfer.

1 Starting the OMNIS Software

- Start the OMNIS Software.

A message appears.

2 Opening the transfer wizard

- In the OMNIS Software, go to the **Settings** ▶ **Software licenses** area and click on **[Transfer software licenses]** to open the transfer wizard.

A dialog is opened.

3 Selecting a transfer type

- Click on **[Continue offline]** to start the offline transfer. Follow the instructions of the transfer wizard.

4 Creating a license request file

- Save the license request file and send the file to the regional Metrohm representative. Follow the instructions of the transfer wizard.

The regional Metrohm representative must validate the license request file online, create a response file, and send it back.

5 License removal

As soon as the regional Metrohm representative has created and returned the corresponding file, click on **[Open file path]**.

Upload the license request file to remove all licenses from the computer.

6 Creating a license request file

- Save the license request file and send the file to the regional Metrohm representative. Follow the instructions of the licensing wizard.

Upload the license request file from the regional Metrohm representative to the new computer.

7 Closing the transfer wizard

- As soon as the **Updated license request file created** dialog appears, close the transfer wizard by clicking on **[Close]**. If several software licenses have been transferred, repeat steps 4 to 6.

If the **System Information Update** license has not been activated, then a dialog will appear after clicking on **[Transfer software licenses]** to the effect that the regional Metrohm representative must be contacted.

See also

Changing the operation mode (chapter 6.1.8, page 1233)

Licenses - Definition (chapter 4.2, page 29)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operation mode – Definition (chapter 6.1.7, page 1233)

User rights – Directory (chapter 4.5.7.4, page 89)

4.2.3 Activating the function license

The OMNIS Software for the operation of the OMNIS instruments is modular in structure. Instrument functions are available as license packages. Some instrument functions can be licensed and activated individually. Included in the purchase of an OMNIS instrument are the functionalities in the respective license package which can be activated following installation and licensing. Additional functions can be obtained and activated later as required. If you have questions about function licenses, contact your regional Metrohm representative.

These instructions only apply for OMNIS instruments. No licensing is needed to use the instrument functions of Metrohm USB instruments.

The activation of function licenses can only be carried out in the Main operation mode. Further information on the operation modes: *Changing the operation mode*

Prerequisite:

- The OMNIS Software is installed.
- The ticket number (format: 12345-12345-ABCDE-ABCDE-1X2Y3) is available.
- The customer number (format: 123-456789) is available.
- The Main operation mode was selected.
- The user has the necessary rights. Additional information on the user rights: *Metrohm Knowledge Base*

1 Opening the instrument management

- Reserve and select the desired instrument under **Equipment ► Instruments**.

2 Displaying instrument functions

- Click on to open the **Properties** window and select the **Licenses and firmware** subsection.

The functions that are activated and not activated on the instrument are displayed in the **Licenses and firmware** subsection.

3 Opening the licensing wizard

- Click on **[Activate function licenses]** to open the licensing wizard.

A dialog is opened.

4 Selecting the type of licensing

- Start online licensing or offline licensing by clicking on **[Continue]** or **[Continue offline]**.
- Follow the instructions of the licensing wizard.

- Online licensing is possible if the computer with the OMNIS Software has direct Internet access.
- Offline licensing must be selected if the computer with the OMNIS Software does not have direct Internet access and therefore another computer with Internet access has to be used. It must be possible to exchange data between both computers, e.g. via a USB flash drive.

The license activation file is loaded onto the OMNIS instrument.

This may take several minutes. Do not exit the OMNIS Software during this process.

5 Closing the licensing wizard

- Once the dialog **The license was successfully activated** appears, close the licensing wizard by clicking on **[Close]**.

The additional instrument functions are now activated.

A function license that is already activated on the computer will also remain in effect in the event of an OMNIS Software update. Contact your regional Metrohm representative in the event that the computer needs to be replaced or exchanged.

See also

Changing the operation mode (chapter 6.1.8, page 1233)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operation mode – Definition (chapter 6.1.7, page 1233)

User rights – Directory (chapter 4.5.7.4, page 89)

4.2.4 Transferring a function license

These instructions apply only for OMNIS instruments. No licensing is needed to use the instrument functions of Metrohm USB instruments.

The transfer of function licenses can be carried out only in Main operation mode. Additional information on the operation modes: *Changing the operation mode*

Prerequisite:

- The OMNIS Software is installed.
- The Main operation mode has been selected.
- The user has the necessary rights. Additional information on the user rights: *Metrohm Knowledge Base*
- Contact your regional Metrohm representative to complete the license transfer.

1 Opening the instrument management

- Reserve and select the desired instrument under **Equipment ▶ Instruments**.

2 Displaying instrument functions

- Click on to open the **Properties** window and select the **Licenses and firmware** subsection.

The function licenses that are activated and not activated on the instrument are displayed in the **Licenses and firmware** subsection.

3 Opening the transfer wizard

- Click on **[Transfer function licenses]** to open the transfer wizard.

Follow the instructions of the transfer wizard.

4 Closing the transfer wizard

As soon as the **Updated license request file generated** dialog appears, follow the instructions of the transfer wizard and close it by clicking on **[Close]**. If several function licenses have been activated, repeat steps 1 to 4.

If the **System Information Update** license has not been activated, then a dialog will appear after clicking on **[Transfer function licenses]** to the effect that the regional Metrohm representative must be contacted.

See also

Changing the operation mode (chapter 6.1.8, page 1233)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operation mode – Definition (chapter 6.1.7, page 1233)

User rights – Directory (chapter 4.5.7.4, page 89)

4.2.5 Software licenses – Subsection

The following functions are available under **Settings** ▶ **Software licenses**:

Activating the software license

- Click on **Continue** to activate the software licenses with the aid of a computer with Internet access.
- Click on **Continue offline** to activate the software licenses with the aid of a computer without Internet access.
  Offline licensing is selected if the computer does not have direct Internet access, for which reason a different computer with Internet access needs to be used. It must be possible to exchange data between the two computers, e.g. via a USB flash drive. Additional information: *(see "Activating the software license", chapter 4.2.1, page 29)*

Transferring a software license

- Click on **Continue** to transfer the software licenses with the aid of a computer with Internet access.

- Click on **Continue offline** to transfer the software licenses with the aid of a computer without Internet access.
  Offline transfer is selected if the computer does not have direct Internet access, for which reason a different computer with Internet access needs to be used. It must be possible to exchange data between the two computers, e.g. via a USB flash drive. This licence transfer can be carried out only with the aid of a regional Metrohm representative.
  Additional information: *(see "Transferring a software license", chapter 4.2.2, page 32)*

4.3 Locking compliance

Information on the settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The functions for **Compliance FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** are shown if the following prerequisites are met:

- A valid (**Compliance/Regulation Stand-Alone** or **Compliance/Regulation Client/Server**) software license is used.
- User management is activated.
- The user has the necessary rights. Further information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

Once compliance is locked, it cannot be unlocked again. Apart from that, the **Audit Trail**, **Signatures** and **Password required** functions can no longer be deactivated. The **Modification comment** function is optional and can be deactivated at any time.

Locking compliance

1 Activating the Audit Trail

- Activate the **Audit Trail** function by clicking on the check box in **Settings** ▶ **Advanced settings**.

The icon for the **Audit Trail** work area is displayed in the navigation bar. The Audit Trail is activated and all the modifications made in the OMNIS Software are recorded.

2 Activating signatures

- Activate the **Signatures** function by clicking on the check box.

The signatures are activated. They allow for a two-step approval process for subsamples, methods and operating procedures. Signed objects are protected against modifications.

3 Activating the "Enforce login with password" function

- In **User management** ▶ **User management settings**, activate the **Password required** function by clicking on the check box.
- Click on to save the changed settings in the user management.

Once this function has been activated, the same **Password required** function is also activated in **Settings** ▶ **Advanced settings** ▶ **Compliance**.

The password of the user must be entered for each login.

4 Locking compliance

- Activate the **[Lock compliance]** function by clicking on the button.

A dialog is opened.

5 Confirming the message

Once compliance is locked, it cannot be unlocked again. Apart from that, the **Audit Trail**, **Signatures** and **Password required** functions can no longer be deactivated.

- Confirm the action by clicking on **[Continue]**.
- Alternatively cancel the action by clicking on **[Cancel]**.

The **Audit Trail**, **Signatures** and **Password required** functions are activated and cannot be deactivated.

Optional

1 Activating the modification comment

- Activate the **Modification comment** function by clicking on the check box.

The **Audit Trail** function is activated automatically. All modifications made in the sample list can be saved only with a comment.

2 Deactivating a modification comment

- Deactivate the **Modification comment** function by clicking on the check box.

The settings **Signatures**, **Password required** and **Modification comment** will only take effect after a restart of the OMNIS Software.

See also

Audit Trail – Actions (chapter 5.14, page 1171)

General settings – Subsection (chapter 5.15.3, page 1203)

Modification comment – Brief description (chapter 5.6, page 192)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Signature – Brief description (chapter 5.8, page 197)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User management settings – Subsection (chapter 4.5.4, page 66)

User rights – Directory (chapter 4.5.7.4, page 89)

4.4 User management (Active Directory) – Actions

Information on the central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

In the event of **user management with Active Directory integration**, the following actions can be carried out in the **User management** work area in the subsections:

-

  The entered Active Directory integration data is changed and all information regarding synchronization with Active Directory is displayed in **User management** ▶ **User management settings**. The security settings can also be managed. Some specifications regarding security settings are applied only to the administrator. The **Automatic locking** and **Password required** settings apply for all users.

-

  All the users are displayed in **User management** ▶ **User list**. New users can no longer be created and edited after activation of the user management with Active Directory integration. New user accounts are created and edited in Active Directory.

-

  All the created user groups are displayed in **User management** ▶ **User groups**. A user group can be selected and edited and new user groups can be created. The **mapping** and thus the assignment to the existing Active Directory group takes place in the properties of a user group. Optionally, data permissions can be assigned to the user groups. These data permissions influence which users can see and edit which data in the OMNIS Software.

-

  Under **User management** ▶ **Data permissions**, data permissions can be set up, activated or deactivated. The deactivation of data permissions can be locked.

-

  New user roles can be created, all existing user roles are managed and user roles are equipped with rights in **User management** ▶ **User roles**. These rights affect what the users in user groups with this user role can view and execute in the OMNIS Software.

See also

Data permissions – Definition (chapter 4.5.9, page 105)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

Managing the password (chapter 4.5.8, page 102)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

User groups – Properties (chapter 4.5.6.2, page 82)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management settings – Subsection (chapter 4.5.4, page 66)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5 User management (OMNIS) – Actions

Information on the central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The following actions can be carried out in the **User management** work area in the subsections using the **User management (OMNIS)**:

-

  The setting-up of user management with Active Directory integration can be started retroactively to the user management (OMNIS) and the security settings can be managed in **User management** ▶ **User management settings**.

-

  Users can be recorded, all recorded users are managed and users are assigned to user groups in **User management** ▶ **User list**.

-

  New user groups can be created, all existing user groups are managed and user groups are linked with user roles in **User management** ▶ **User groups**. Optionally, data permissions can be assigned to the user groups. These data permissions influence which users can see and edit which data in the OMNIS Software.

-

  Under **User management** ▶ **Data permissions**, data permissions can be set up, activated or deactivated. The deactivation of data permissions can be locked.

-

  New user roles can be created, all existing user roles are managed and user roles are equipped with rights in **User management** ▶ **User roles**. These rights affect what the users in user groups with this user role can view and execute in the OMNIS Software.

See also

Data permissions – Definition (chapter 4.5.9, page 105)

Managing the password (chapter 4.5.8, page 102)

Managing the password (chapter 4.5.8, page 102)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

User groups – Properties (chapter 4.5.6.2, page 82)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management settings – Subsection (chapter 4.5.4, page 66)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.1 User management – Definition

Two types of user management are available in the OMNIS Software:

- **Active Directory:** This is an external user management, a directory service from Microsoft. User management can be set up in the OMNIS Software with a connection to Active Directory. This link uses the Active Directory infrastructure in that already existing user accounts and groups are accessed. The user has the possibility of authenticating himself or herself in the OMNIS Software in the future using his or her Active Directory user account. The assignment of user rights to user roles and the assignment of user roles and data permissions (optional) to user groups remains within the OMNIS Software.

  Metrohm recommends setting up **User management with Active Directory integration**, as this type of user management has significantly more integrated security features than the internal **User management (OMNIS)**.

  There are 2 possible ways to set up user management with Active Directory integration: Either initially at the time user management is set up or retroactively, if the **User management (OMNIS)** has already been activated.

- **User management (OMNIS):** This is an internal user management which is integrated in the OMNIS Software. User accounts, user groups and user roles are created and edited within the OMNIS Software by an administrator. The administrator also assigns the necessary user rights. Optionally, data permissions can be assigned to the user groups.

It is a prerequisite to enable the user management when using the **OMNIS Client/Server system**. All the settings that were made in the user management are valid in the **OMNIS Client/Server system** for all the connected OMNIS Clients (central user management).
Additional information on central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

See also

Data permissions – Definition (chapter 4.5.9, page 105)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User list – Definition (chapter 4.5.5.1, page 70)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User management settings – Subsection (chapter 4.5.4, page 66)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

4.5.2 Enabling user management (Active Directory)

The activation of the **user management with Active Directory integration** should never be carried out in the OQ-FS operation mode.

User management with Active Directory integration is an external user management based on a directory service from Microsoft. This Active Directory service from Microsoft can be used to link the OMNIS Software and the Active Directory to one another. Existing Active Directory user accounts and Active Directory user groups can thus be used in the OMNIS Software. Azure Active Directory, the cloud-based version of the directory service, cannot be integrated into the OMNIS Software at the moment.

Active Directory	Supported	Not supported
Microsoft Active Directory	X	
Microsoft Azure Active Directory		X

There are 2 options to set up user management with Active Directory integration:

- *Option 1:* To begin with when setting up user management.
- *Option 2:* First, enable the local user management (OMNIS) and then set up the Active Directory integration.

An enabled user management is a prerequisite for the following functions:

OMNIS Client/Server system: A corresponding message shows that the user management must be enabled directly after the first OMNIS Client has been set up. Additional information: *OMNIS Client/Server system – Definition*

3rd Party Data Integration API: Additional information: *Data exchange with third-party software – Definition*

Data permissions: Additional information: *Data permissions – Definition*

The user management with Active Directory integration cannot be disabled again for traceability reasons.

In both cases, successful setup depends on the specification of **Domain**, **User name**, **Password** and **Distinguished Name** or **Synchronization group** as the first step. An assignment of a user group to an existing Active Directory group must take place in the following step. This **mapping** causes user groups and user roles to be assigned to Active Directory users who belong to the respective user group in the OMNIS Software. The user rights must be specified in the OMNIS Software following successful **synchronization** of the Active Directory user accounts. Synchronization takes place every 12 hours and each time the computer is restarted. The function of a manual synchronization also exists in the OMNIS Software.

Active Directory settings can be changed retroactively following successful setup: *Changing the connection settings*

Option 1

Prerequisite:

- The OMNIS Software is installed.
- The required operation mode was selected.
  Additional requirements for OMNIS Client/Server system:

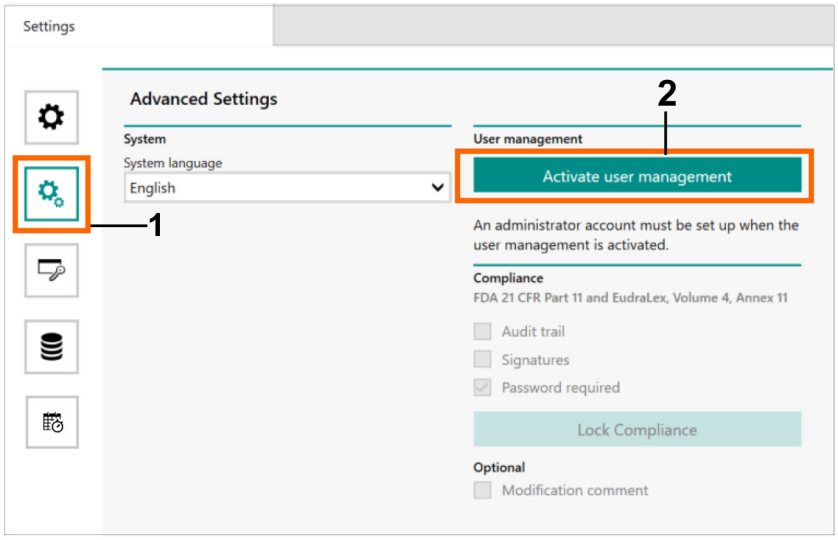
- The first OMNIS Client was added to the **OMNIS Client/Server system**.

1 Enabling user management

This step only applies to **OMNIS Stand-Alone**.

If there are unsaved changes or running determinations, the user management cannot be enabled. Changes must be saved beforehand and ongoing determinations must be ended or stopped.

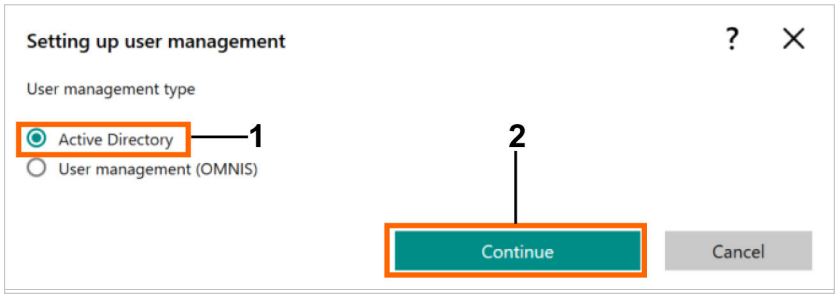
- Open the OMNIS Software.
- In **Settings** ▶ **Advanced settings** ▶ **User management** (**1**), click on **[Activate user management]** (**2**).



A dialog is opened.

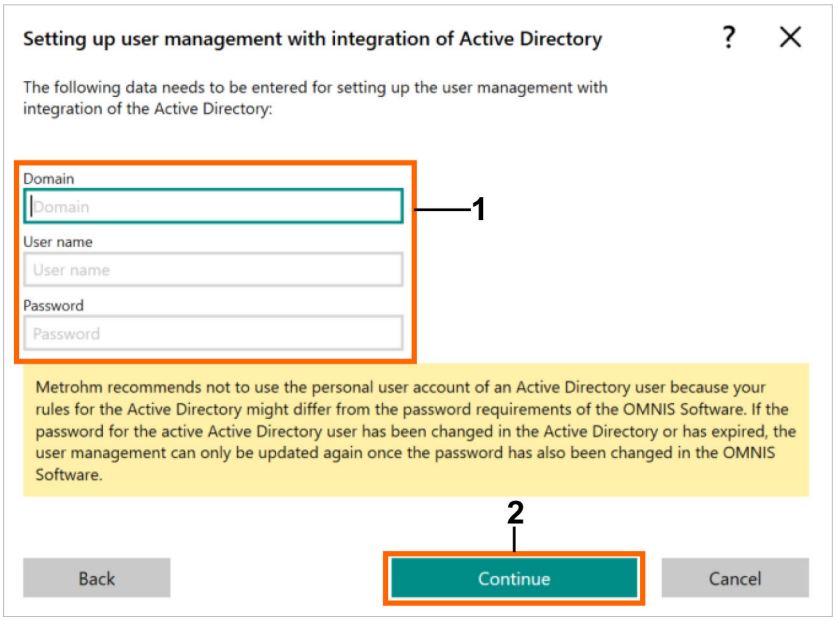
2 Selecting the user management type

- Select the **Active Directory** type of user management (**1**).
- Start the setup by clicking on **[Continue]** (**2**).



3 Entering domain, user name and password

- Enter **Domain**. For a secure connection, add the port number 636 with the domain. Example: domainname:636 (**1**).
- Enter **User name** and **Password** (**1**).
- Click on **[Continue]** (**2**) to continue the setup.



The specification of a user name is required for Active Directory access and for later synchronization between OMNIS Software and Active Directory. This user requires a read permission for the domain.

Metrohm does not recommend using the personal user account of an Active Directory user because the rules for the Active Directory might differ from the password guidelines of the OMNIS Software. If the password for the used Active Directory user has been changed in the Active Directory or has expired, then the user management can no longer be updated until the password has also been changed in the OMNIS Software.

4 Creating the synchronization group in the Active Directory

- Open the Active Directory (e.g. the LDAP browser of Softerra or the Active Directory of Microsoft Windows).
- Create a synchronization group. The name of the synchronization group is freely selectable (e.g. Sync group) (**1**).

- Right-click on the synchronization group and select **Properties** in the selection list. Add all existing Active Directory groups of the synchronization group on the **Members** tab (**2**).

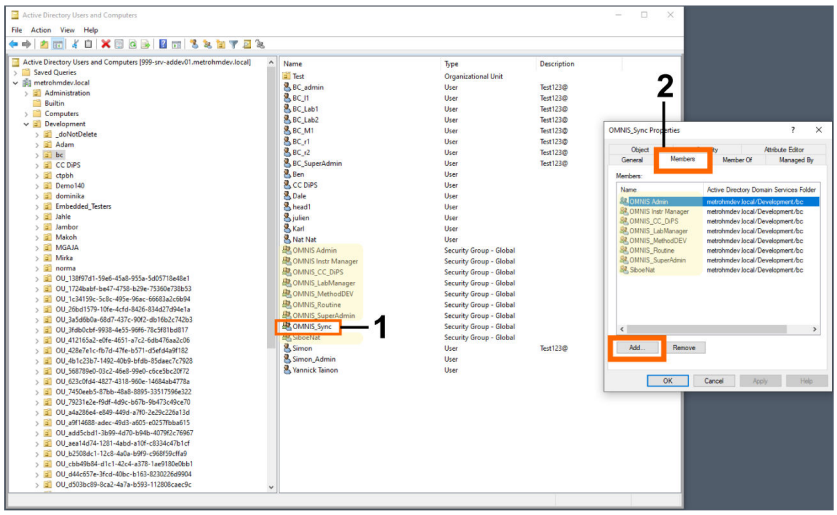


Figure 1 Example for Active Directory of Microsoft Windows

The synchronization group is the only Active Directory group (domain) that will later be connected to the OMNIS Software. The synchronization group must contain all Active Directory groups (e.g. laboratory managers, routine users, ...) as members that are to be synchronized later with the OMNIS Software. All Active Directory users are located in the Active Directory groups (e.g. laboratory managers, routine users, ...).

5 Copying the Distinguished Name of the synchronization group

- Right-click on the synchronization group and select **Properties** in the selection list.
- Under **Attribute editor**, select the **DN (Distinguished Name)** (**1**).
- Copy the complete path.

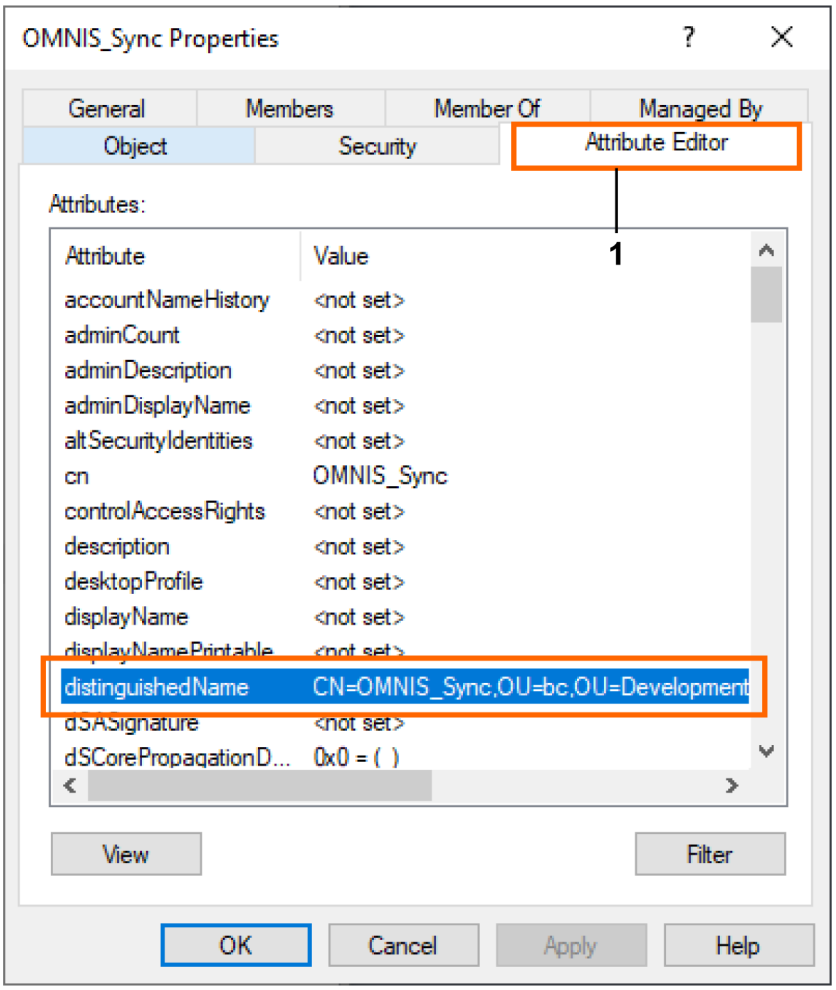
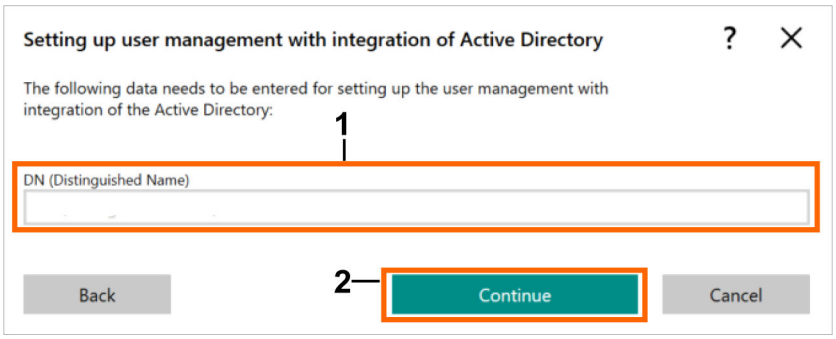


Figure 2 Example for Active Directory of Microsoft Windows

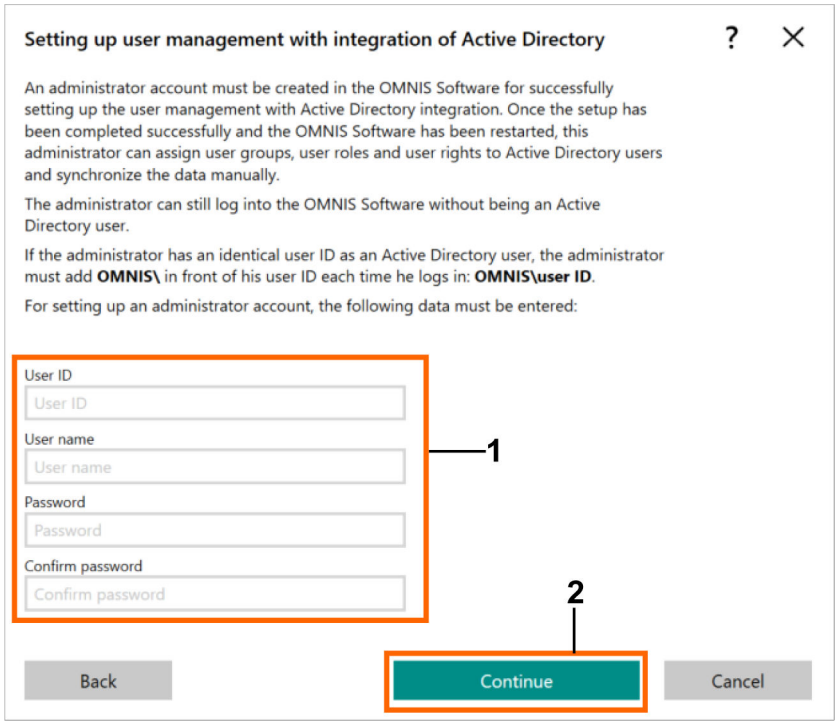
6 Entering the Distinguished Name of the synchronization group

- Enter the previously copied **DN (Distinguished Name)** (**1**).
- Click on **[Continue]** (**2**) to continue the setup.



7 Setting up an administrator account

- Define **User ID**, **User name**, **E-mail address** and **Password** for the administrator account (**1**).
- Click on **[Continue]** (**2**) to continue the setup.



If access to the OMNIS Software is not possible, then it will also not be possible to reset the password. Metrohm therefore recommends that the **User ID** and the **Password** be noted down as well.

8 Confirming the setup

- For activation of the user management with Active Directory integration, click on **[Close OMNIS Software]**.

9 Restarting the OMNIS Software

- Start the OMNIS Software as an administrator.

If the administrator has the same user ID as an Active Directory user, then the administrator must place **OMNIS** before his or her user ID at the time of each login: **OMNIS\user ID**. Otherwise the Active Directory user will be detected instead of the administrator.

The icon for the **User management** work area is displayed in the navigation bar.

In the **OMNIS Client/Server system**, the OMNIS Software does not need to be restarted after the user management with Active Directory integration has been set up successfully.

10 Opening a user group

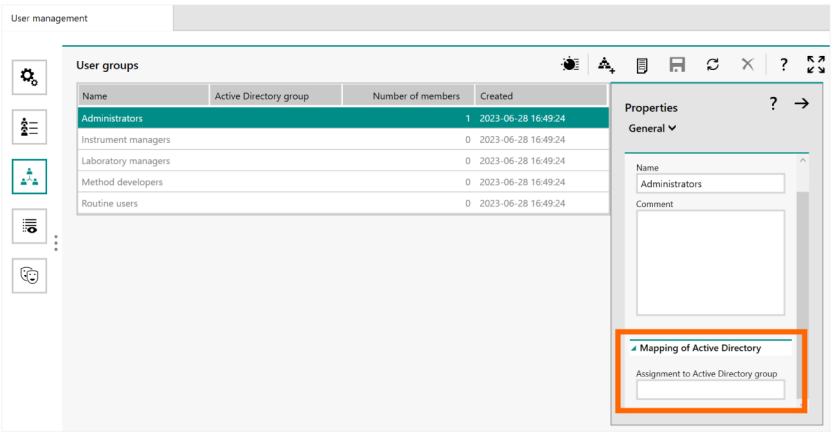
- Select a user group in **User management** ▶ **User groups** or create a new user group by clicking on .
- Open the settings for the selected or newly created user group by clicking on .

11 Copying the Distinguished Name of the Active Directory group

- In Active Directory, select the Active Directory group to be connected to the OMNIS Software.
- Right-click on the Active Directory group and select **Properties** in the selection list.
- Under **Attribute editor**, select the **DN (Distinguished Name)**.
- Copy the complete path.

12 Assignment to Active Directory group

- Under **User management** ▶ **User groups** ▶ **Properties** ▶ **Mapping of Active Directory** ▶ **Assignment to Active Directory group**, insert the previously copied **DN (Distinguished Name)** of the Active Directory group.

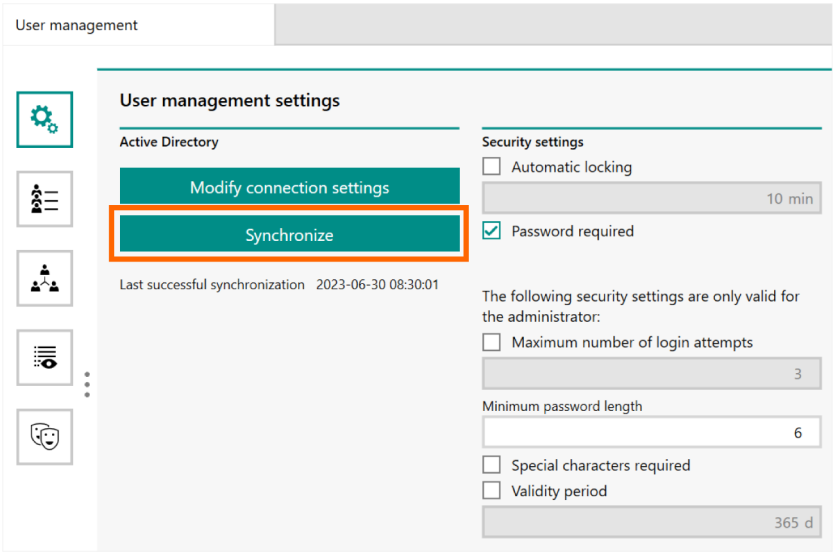


13 Saving changes

- Click on to save the data entered.

14 Manual synchronization

- Start the synchronization with Active Directory by clicking on **[Synchronize]** in **User management ▶ User management settings**.



15 Updating a user list

- Update the user list by clicking on in **User management ▶ User list**.

The **User groups** and **User roles** columns are filled in.

Repeat steps 10 to 15 for all the relevant user groups. The OMNIS Software can then be used with the settings used in the Active Directory.

16 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

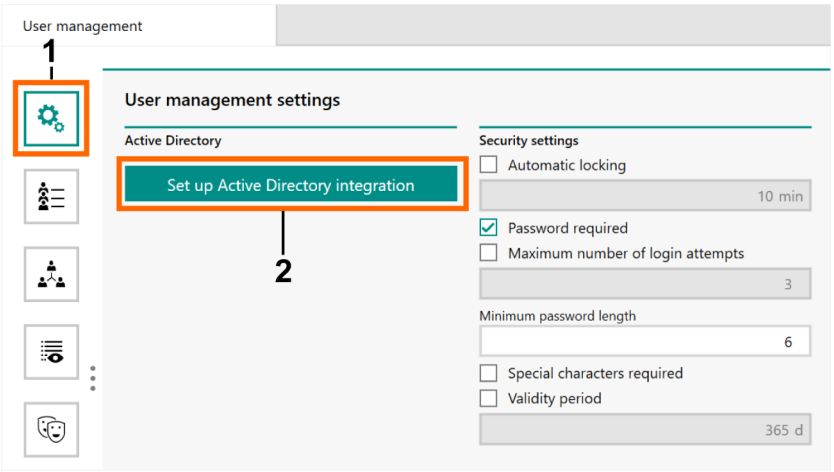
Option 2

Prerequisite:

- User management (OMNIS) is activated.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory*
- The required operation mode was selected.

1 **Retroactive integration of Active Directory**

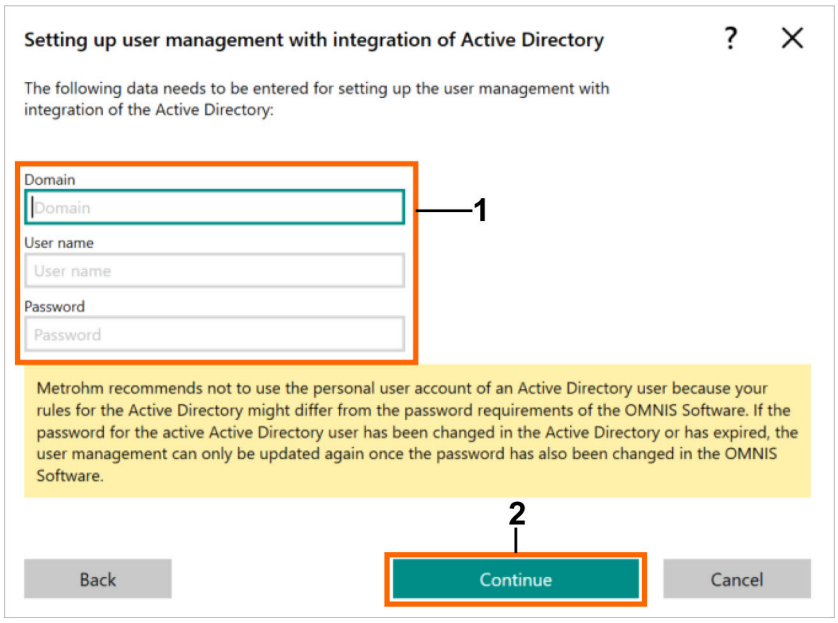
- In **User management** ▶ **User management settings** (**1**), click on **[Set up Active Directory integration]** (**2**).



A dialog is opened.

2 **Entering domain, user name and password**

- Enter **Domain**. For a secure connection, add the port number 636 with the domain. Example: domainname:636 (**1**).
- Enter **User name** and **Password** (**1**).
- Click on **[Continue]** (**2**) to continue the setup.



Metrohm does not recommend using the personal user account of an Active Directory user because the rules for the Active Directory might differ from the password guidelines of the OMNIS Software. If the password for the used Active Directory user has been changed in the Active Directory or has expired, then the user management can no longer be updated until the password has also been changed in the OMNIS Software.

3 Creating the synchronization group in the Active Directory

- Open the Active Directory (e.g. the LDAP browser of Softerra or the Active Directory of Microsoft Windows).
- Create a synchronization group. The name of the synchronization group is freely selectable (e.g. Sync group) (**1**).
- Right-click on the synchronization group and select **Properties** in the selection list. Add all existing Active Directory groups of the synchronization group on the **Members** tab (**2**).

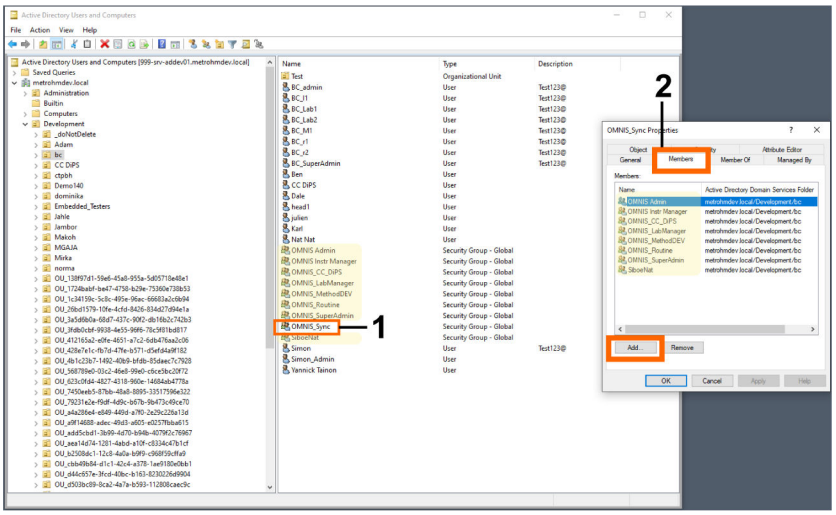


Figure 3 Example for Active Directory of Microsoft Windows

The synchronization group is the only Active Directory group (domain) that will later be connected to the OMNIS Software. The synchronization group must contain all Active Directory groups (e.g. laboratory managers, routine users, ...) as members that are to be synchronized later with the OMNIS Software. All Active Directory users are located in the Active Directory groups (e.g. laboratory managers, routine users, ...).

4 Copying the Distinguished Name of the synchronization group

- Right-click on the synchronization group and select **Properties** in the selection list.
- Under **Attribute editor**, select the **DN (Distinguished Name)** (**1**).
- Copy the complete path.

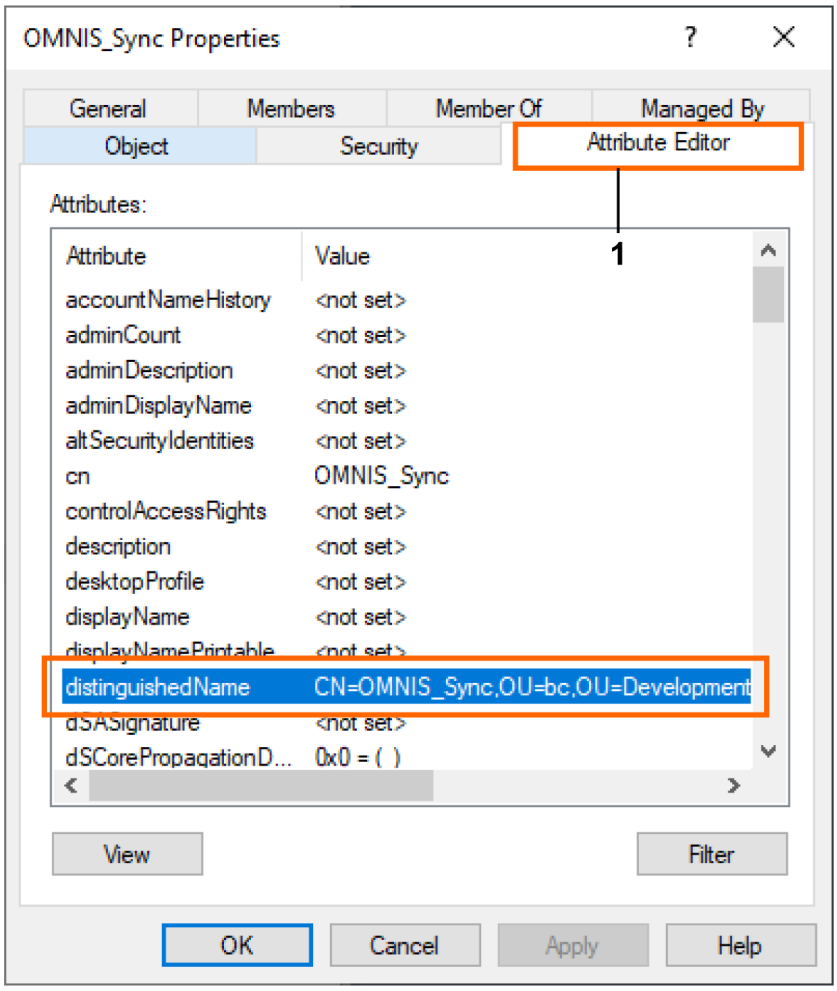
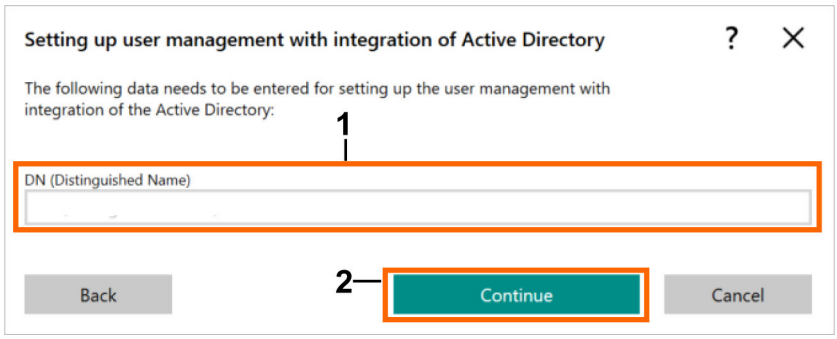


Figure 4 Example for Active Directory of Microsoft Windows

5 Entering the Distinguished Name of the synchronization group

- Enter the previously copied **DN (Distinguished Name)** (**1**).
- Click on **[Continue]** (**2**) to continue the setup.



6 Confirming the setup

- For activation of the user management with Active Directory integration, click on **[Close OMNIS Software]**.

7 Restarting the OMNIS Software

- Start the OMNIS Software as an administrator.

If the administrator has the same user ID as an Active Directory user, then the administrator must place **OMNIS** before his or her user ID at the time of each login: **OMNIS\user ID**. Otherwise the Active Directory user will be detected instead of the administrator.

The user accounts that were previously created in the user management (OMNIS) are all disabled except the administrator account that was last created. New user accounts must be created exclusively through Active Directory.

8 Opening a user group

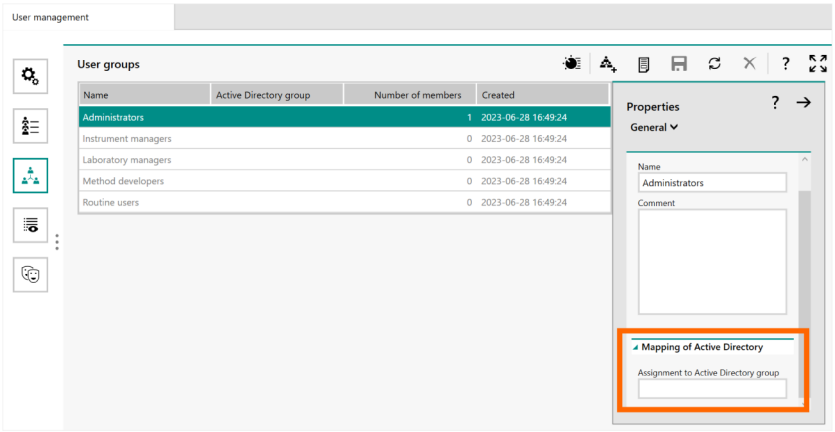
- Select a user group in **User management** ▶ **User groups** or create a new user group by clicking on .
- Open the settings for the selected or newly created user group by clicking on .

9 Copying the Distinguished Name of the Active Directory group

- In Active Directory, select the Active Directory group to be connected to the OMNIS Software.
- Right-click on the Active Directory group and select **Properties** in the selection list.
- Under **Attribute editor**, select the **DN (Distinguished Name)**.
- Copy the complete path.

10 Assignment to Active Directory group

- Under **User management** ▶ **User groups** ▶ **Properties** ▶ **Mapping of Active Directory** ▶ **Assignment to Active Directory group**, insert the previously copied **DN (Distinguished Name)** of the Active Directory group.

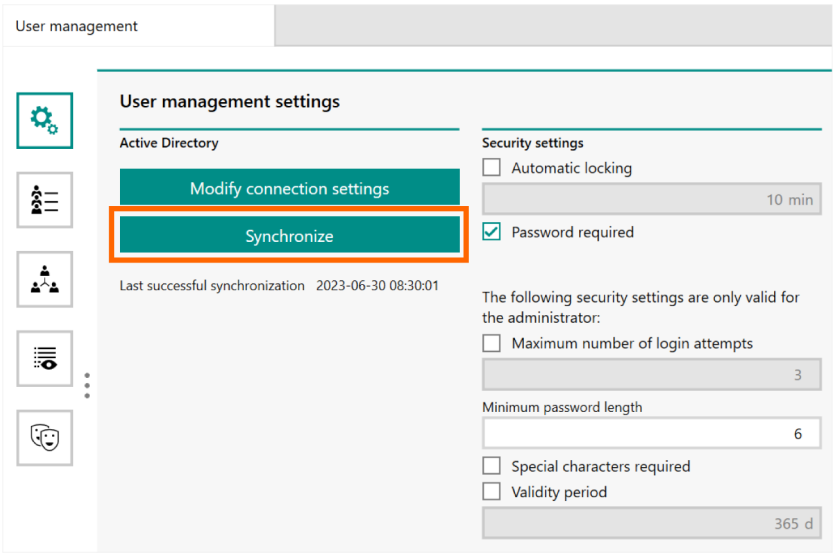


11 Saving changes

- Click on to save the data entered.

12 Manual synchronization

- Start the synchronization with Active Directory by clicking on **[Synchronize]** in **User management** ▶ **User management settings**.



13 Updating a user list

- Update the user list by clicking on in **User management** ▶ **User list**.

The **User groups** and **User roles** columns are filled in.

Repeat steps 8 to 13 for all the relevant user groups. The OMNIS Software can then be used with the settings used in the Active Directory.

14 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

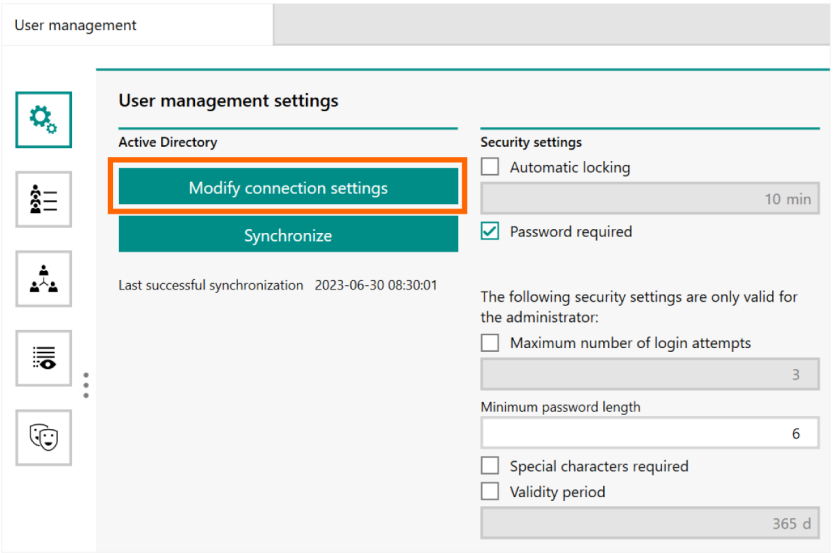
Modifying the connection settings

Prerequisite:

- User management with Active Directory integration is activated.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory*
- The required operation mode was selected.

1 Modifying data

- Click on **[Modify connection settings]** in **User management ▶ User management settings** to change the entered data of the Active Directory integration.

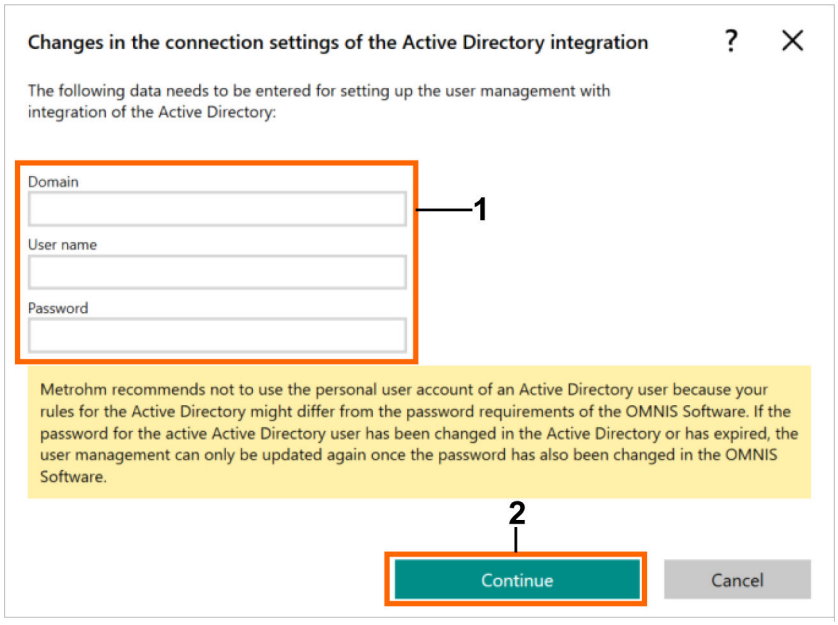


A dialog with pre-filled input fields opens.

2 Entering domain, user name and password again

- Enter **Domain**. For a secure connection, add the port number 636 with the domain. Example: domainname:636 (**1**).
- Enter **User name** and **Password** (**1**).

- Click on **[Continue]** (**2**) to continue the setup.

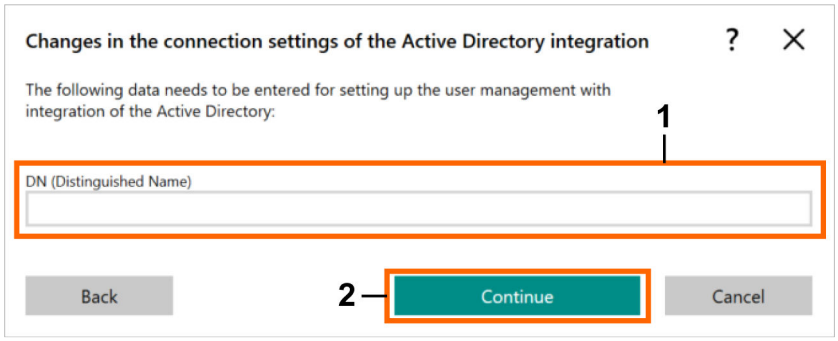


Metrohm does not recommend using the personal user account of an Active Directory user because the rules for the Active Directory might differ from the password guidelines of the OMNIS Software. If the password for the used Active Directory user has been changed in the Active Directory or has expired, then the user management can no longer be updated until the password has also been changed in the OMNIS Software.

A dialog is opened.

3 Entering the Distinguished Name of the synchronization group again

- Change the **DN (Distinguished Name)**, if necessary (**1**).
- Click on **[Continue]** to continue changing the data (**2**).

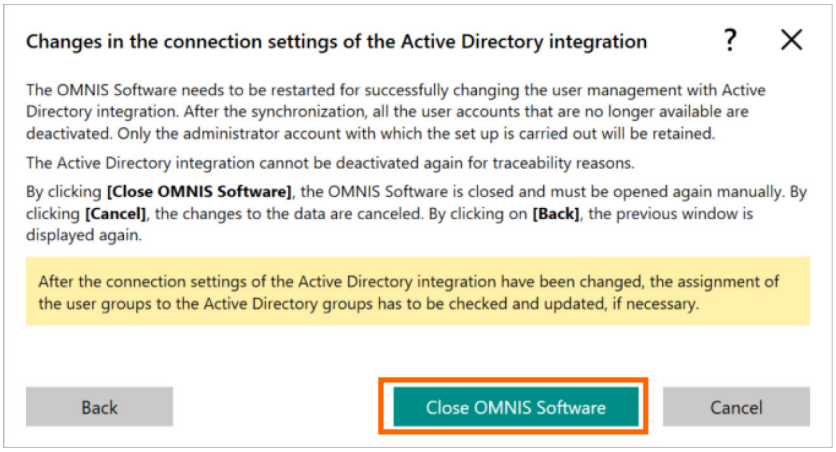


If the **Domain** was changed in the previous dialog, then the **DN (Distinguished Name)** also must be changed. In this case, the **DN (Distinguished Name)** input field is not pre-filled.

A dialog is opened.

4 Confirming the changed data

- Confirm the changed data and restart the OMNIS Software by clicking on **[Close OMNIS Software]**.



After the connection settings of the Active Directory integration have been changed, the assignment of the user groups to the Active Directory groups has to be checked, and updated if necessary.

5 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

See also

Changing the operation mode (chapter 6.1.8, page 1233)

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Data permissions – Definition (chapter 4.5.9, page 105)

Managing the password (chapter 4.5.8, page 102)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Operation mode – Definition (chapter 6.1.7, page 1233)

User groups – Definition (chapter 4.5.6.1, page 81)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

4.5.3 Enabling user management (OMNIS)

To perform service activities, a total of 3 operation modes of the OMNIS system must be configured. The activation of the **user management (OMNIS)** must be carried out for each operation mode separately.

User management (OMNIS) is an internal user management which is integrated in the OMNIS Software. All the user accounts, user groups and user roles are created and edited with a newly created administrator account within the OMNIS Software. This administrator also assigns the necessary rights. Data permissions can optionally be assigned to the user groups.

An enabled user management is a prerequisite for the following functions:

OMNIS Client/Server system: A corresponding message shows that the user management must be enabled directly after the first OMNIS Client has been set up. Additional information: *OMNIS Client/Server system – Definition*

3rd Party Data Integration API: Additional information: *Data exchange with third-party software – Definition*

Data permissions: Additional information: *Data permissions – Definition*

Prerequisite:

- The OMNIS Software is installed.
- The required operation mode was selected.

Additional requirements for OMNIS Client/Server system:

- The first OMNIS Client was added to the **OMNIS Client/Server system**.

1 Enabling user management (OMNIS)

This step only applies to **OMNIS Stand-Alone**.

If there are unsaved changes or running determinations, the user management cannot be enabled. Save changes first and end or stop running determinations.

- In **Settings** ▶ **Advanced settings** ▶ **User management**, click on **[Activate user management]**.

A dialog is opened.

2 Selecting the user management type

- Select the **User management (OMNIS)** type of user management.
- Start the setup by clicking on **[Continue]**.

The setting-up of the user management (OMNIS) is started.

3 Setting up an administrator account

- Define **User ID**, **User name** and **Password** for the administrator account.

The first user is automatically assigned to the **Administrators** user group.

The new settings will only take effect after a restart of the OMNIS Software.

If the user management with Active Directory integration is activated retroactively and if the administrator has the same user ID as an Active Directory user, then the administrator must place **OMNIS** before his or her user ID at the time of each login: **OMNIS\user ID**. Otherwise the Active Directory user will be detected instead of the administrator.

The entries made are applied by clicking on **[Continue]**.

4 Confirming the setup and restarting OMNIS Software

- For activation of the user management (OMNIS), click on **[Close OMNIS Software]** and then restart the OMNIS Software manually.

The new settings will only take effect after a restart of the OMNIS Software.

Login with the previously defined data is necessary after restarting the OMNIS Software.

User management cannot be deactivated again once it has been activated due to reasons of traceability.

The icon for the **User management** work area is displayed in the navigation bar.

In the **OMNIS Client/Server system**, the OMNIS Software does not need to be restarted after the user management (OMNIS) has been set up successfully.

5 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

The administrator creates user accounts and defines passwords for the users:

1 Creating a new user

- In **User management** ▶ **User list**, click on .

An empty line for the new user appears in the user list.

2 Defining a password

- Click on to open the **Properties** for the selected user.
- Under **Properties** ▶ **General**, fill out the required fields **User ID** and **User name**, define the **Password** and announce this to the user.
- Click on to save the data entered.

Users must change their passwords at the time of first login. Only users with administrator rights can create new users and define their passwords.

If the user has forgotten his or her password, then the administrator can reset that user's password:

1 Resetting a password

- Under **User management** ▶ **User list**, select the user.
- Click on to open the **Properties** for the selected user.
- Enable the **[Reset password]** check box.
- Define a new password and confirm it with a second entry.

- Click on to save the data entered.

Only users with administrator rights can reset passwords.
If the administrator forgets his or her own password or if the validity period of his or her password expires, then there is no possibility of resetting the password on one's own. Please contact your regional Metrohm representative in such cases.

If the **Audit Trail** function in the **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** option is activated, then all of the changes made in the OMNIS Software will be recorded and listed in the Audit Trail.

See also

Changing the operation mode (chapter 6.1.8, page 1233)

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Data permissions – Definition (chapter 4.5.9, page 105)

Managing the password (chapter 4.5.8, page 102)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Operation mode – Definition (chapter 6.1.7, page 1233)

User groups – Definition (chapter 4.5.6.1, page 81)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

4.5.4 User management settings – Subsection

Information on the central management of the security settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The following settings for Active Directory and for the security settings are available in **User management** ▶ **User management settings**:

Active Directory

- User management with Active Directory integration can be set up retroactively with **[Set up Active Directory integration]**, if the user management (OMNIS) has already been activated.

More information on setting up user management with or without Active Directory integration: *(see "Enabling user management (Active Directory)", chapter 4.5.2, page 45), (see "Enabling user management (OMNIS)", chapter 4.5.3, page 63)*

All previously existing user accounts are deactivated after the successful setting up of the Active Directory integration. Only the administrator account under which the setup was carried out remains in existence in the OMNIS Software.

If this administrator deactivates the right **Manage users**, then he or she will lose access to the user management. Only Active Directory users who were previously equipped by the administrator with administrator rights can still adjust settings in the user management. Metrohm recommends therefore defining at least one other administrator in the OMNIS Software who is listed in the Active Directory.

- With **[Modify connection settings]**, the Active Directory integration data entered can be changed. After the synchronization, all the user accounts that are no longer available are deactivated.
- With **[Synchronize]**, the synchronization can be started manually and at any time. Date and time of the last successful synchronization are displayed here. Automatic synchronization takes place every 12 hours.

Security settings

Only users with the **Manage users** right can configure the security settings.

In the event of enabled user management with Active Directory integration, some specifications regarding security settings (**Maximum number of login attempts**, **Minimum password length**, **Special characters required**, **Validity period**) are applied only to the administrator. The **Automatic locking** and **Password required** settings apply for all users.

For security reasons, Metrohm recommends always enabling the check boxes for **Automatic locking**, **Maximum number of login attempts** and **Minimum password length**.

- **Automatic locking**: This check box defines the time in minutes until the OMNIS Software is locked automatically after the last user activity (operation of the keyboard or the mouse).

The following settings are available for the **Password administration**:

- **Password required**: This check box forces a user to log in with a password.
  If the check box has been disabled and is enabled again, the check box for **Reset password** must be enabled for each user that was created without a password in **Properties**. Users for whom this is not done can no longer log into the OMNIS Software. *(see "Managing the password", chapter 4.5.8, page 102)*
  If compliance is locked in **Settings** ▶ **Advanced settings**, the **Password required** check box can no longer be enabled or disabled.

To prevent improper access to data, Metrohm recommends never disabling this check box when using the Web API **3rd Party Data Integration API**.

- **Maximum number of login attempts**: This check box defines the number of login attempts. The user is deactivated if this is exceeded and the administrator must enable the user again.
- **Minimum password length**: This check box defines the minimum required character length for the password. The **Password required** check box must be enabled for this.
- **Special characters required**: This check box specifies the use of special characters in the password.
- **Validity period**: This check box defines the expiry time in days, after which a password must be replaced.
  If the **Password never expires** check box is enabled in the properties of a user under **User management** ▶ **User list**, the user's password will never expire, even if a validity period has been defined.

Active Directory passwords are managed in Active Directory and cannot be changed in the OMNIS Software. Additional information on password administration: *(see "Managing the password", chapter 4.5.8, page 102)*

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

If the **Audit Trail** function in the **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** option is activated, then all of the changes made in the OMNIS Software will be recorded and listed in the Audit Trail. Changes which are undertaken directly in the Active Directory are not recorded in the Audit Trail. For additional information regarding the recording of entries in the Audit Trail, see: *(see "Audit Trail – Directory", chapter 5.14.5, page 1177)*

See also

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Locking compliance (chapter 4.3, page 39)

Managing the password (chapter 4.5.8, page 102)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

User groups – Properties (chapter 4.5.6.2, page 82)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.5 User list – Subsection

The following functions are available in **User management** ▶ **User list**:

-

  Use **Create user** to create a new user for which user data can be defined and edited.
-

  Use **Create report** to create a report for the selected user. The report can be saved as a PDF file or printed out.
-

  Use **Save** to save all changes.
-

  Use **Update view** to update the list of the users. All entries are reloaded.
-

  The properties of the selected element are displayed in the **Properties** window.

Overview list

The following information is displayed in the overview list:

User ID	Clear designation which was defined when registering the user.
User name	Name of the user.

User status	Status of the user that can be changed in the properties.
User groups	User groups which were assigned to the user.
User roles	User roles which were assigned to the user groups.
Last login	Date and time of the last login.

See also

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User management – Definition (chapter 4.5.1, page 44)

4.5.5.1 User list – Definition

The following actions can be triggered in **User management** ▶ **User list**, depending on the type of user management that is activated:

New users can be created, existing users can be edited and users can be assigned to user groups in the **User management (OMNIS)**.

For traceability reasons, existing users cannot be deleted again.

All of the synchronized users are displayed in the **User management with Active Directory integration**.

After activating the user management with Active Directory integration, no users can be created and edited in the OMNIS Software. All previously existing user accounts are deactivated after the successful setting up of the user management with Active Directory integration. Only the administrator account under which the setup was carried out remains in existence and can be edited. New users are created exclusively through Active Directory and can be assigned to Active Directory groups. After a restart of the OMNIS Software, the **mapping** of the Active Directory groups with the predefined or newly created user groups takes place in the properties in **User management** ▶ **User groups**.

In the **OMNIS Client/Server system**, the administrator can log into the OMNIS Software in the last dialog of the setup without restarting and carry out the **mapping**. Additional information on central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

If the administrator forgets his or her own password, if he or she has exceeded the maximum number of login attempts or has deactivated the **Manage users** right, then there is no possibility of that person resetting his or her password on their own. The regional Metrohm representative must be contacted in such cases. Additional information on password administration: *(see "Managing the password", chapter 4.5.8, page 102)*

See also

Managing the password (chapter 4.5.8, page 102)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

User groups – Properties (chapter 4.5.6.2, page 82)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Properties (chapter 4.5.5.2, page 72)

User list – Subsection (chapter 4.5.5, page 69)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.5.2 User list – Properties

Information on the central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Clicking on under **User management** ▶ **User list** opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 2 subsections **General** and **User groups**:

General

If the **user management with Active Directory integration** was activated, then the entire area can be viewed by the user, but it cannot be edited, as the data is taken from the Active Directory. The entire area remains editable for the administrator.

The following functions are available to the user of the **user management (OMNIS)** in this subsection:

User ID	Entry of the mandatory entry user ID, which is necessary every time you log into the OMNIS Software. When creating a new user account, a clear and unique user ID needs to be defined which can no longer be changed after saving. The user ID must not contain any of the following special characters: / \ ? * % ; ' " : | [ ] + = < > , The special character @ is only allowed if it appears between part of a text and a domain name, for example: email@example.com Only users with the right to **Manage users** can register new users and define a user ID.
User name	Entry of the mandatory data user name. The user name must consist of the first name and last name and can be retrospectively changed.
E-mail address	Entry of user's e-mail address. The entry is optional and can be changed retrospectively.
Object ID	Object ID of user is displayed. The user is clearly identified with the object ID and the user ID.

User status	The user status can be changed using the check box. The selected status is displayed in the user list with **Active** or **Deactivated**. An inactive user is showed grayed out in the user list and can no longer log into the OMNIS Software.
Reset password	The check box allows the administrator to reset a user's password and define a new password for the user. After logging in with the password defined by the administrator, the user can set his or her own password. **Note:** This check box can be enabled only for existing users.
Password never expires	The check box allows the administrator to specify that a user's password will never expire, even if a password expiry time has been defined in the security settings. Metrohm recommends enabling this check box for the user who is used to access via the Web API (e.g. Technical User). Further information: *(see "Data exchange with third-party software – Definition", chapter 4.9, page 147)*
Request change of password	The check box allows the administrator to request a change of the current password from an existing user. The user will not receive a new password from the administrator for this change of password. The user himself must define and confirm a new password the next time he logs in to the OMNIS Software. For newly created users, this check box is enabled by default so that they receive a password from the administrator for the first-time login, which they can then change. Metrohm recommends disabling this check box for the user who is used to access via the Web API (e.g. Technical User). Further information: *(see "Data exchange with third-party software – Definition", chapter 4.9, page 147)*
Password	For newly created users, the administrator must define and confirm a password. An enabled check box for **Reset password** enables the two input fields for a new password.

Comment	Enter comments about the user. A maximum of 255 characters are allowed in the comment field.

User groups

In this subsection, the OMNIS user or Active Directory user can be assigned to various user groups. Unless they have been assigned to a user group, users will see only the OMNIS Software without data when they log in.

The following pre-defined user groups are available: *(see "User groups – Directory", chapter 4.5.6.3, page 84)*

See also

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Locking compliance (chapter 4.3, page 39)

Managing the password (chapter 4.5.8, page 102)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

User groups – Definition (chapter 4.5.6.1, page 81)

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User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.5.3 Managing users

Information on the central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

To create new users, the **User management (OMNIS)** must be enabled and an administrator account must be set up first. Once the setup of the user management was completed successfully and the OMNIS Software

was restarted, this administrator can log into the OMNIS Software and then create other users.

1 Enabling user management (OMNIS)

- Under **Settings** ▶ **Advanced settings**, click on **[Activate user management]** and enable the **User management (OMNIS)**.
- Enter the following data for the first local user: **User ID**, **User name** and **Password**.

If there are unsaved changes or running determinations, the user management cannot be enabled. Changes must be saved beforehand and ongoing determinations must be ended or stopped.

- The User ID may only be assigned once and must not contain any of the following special characters: / \ ? * % ; ' " : | [ ] + = < > ,
  The special character @ is only allowed if it appears between part of a text and a domain name, for example: email@example.com
- The User name must consist of the first name and last name.
- The Password must be between 6 and 64 characters long. The requirements of the password can be changed after activating user management.
- The first user that is created is automatically assigned to the **Administrators** user group and is therefore assigned the rights of the **Administrator** user role.

- Close the OMNIS Software and restart it. When restarting, it is necessary to login with the defined data.

In the **OMNIS Client/Server system**, the administrator can log into the OMNIS Software without restarting in the last dialog of the setup. Further information on the central user management and the settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

User management cannot be deactivated again due to reasons of traceability.

The icon for the **User management** work area is displayed in the navigation bar.

2 Creating a new user

- Click on under **User management** ▶ **User list** to create a new user that then appears in the user list.
- Select the entry for the new user in the user list and open the properties by clicking on .
- Define the following data for the new user: **User ID**, **User name**, **Password**, **E-mail address** (optional) and **Comment** (optional).

For new users, the **Request change of password** check box is selected by default so that the user receives a password from the administrator for the first-time login, which he can then change. The **Password never expires** check box is disabled in the default setting. The administrator can enable the check box if necessary (e.g. for using the web API by a third-party software) to specify that the user's password will never expire. This also applies if an expiry time for the password has been defined in the security settings.

- Click on to save the data entered.

The newly created user appears as an entry in the user list.

For traceability reasons, a user cannot be deleted but only disabled.

The user registered is automatically a member of the **Routine users** user group. This assignment can be changed.

3 Assigning users to user groups

- Select a user and open the properties by clicking on under **User management** ▶ **User list**.
- Select the **User groups** in the properties of the user.
- Select all required user groups.
- Click on to save the data entered.

The user is added to the user groups as a member.

4 Assigning user roles to a user group

- Select a user group and open the properties by clicking on under **User management** ▶ **User groups**.
- Select the **User roles** in the properties of the user group.

- Select all required user roles.
- Click on to save the data entered.

The selected user roles with their rights are assigned to all members of the user group.

5 Assigning data permissions to the user group (optional)

- Assign data permissions to the user groups according to the following instructions: *(see "Assigning data permissions", chapter 4.5.9.2, page 112)*

6 Equipping user roles with user rights

- Select a user role and open the properties by clicking on under **User management** ▶ **User roles**.
- Select the **User rights** in the properties of the user role.
- Select all required user rights.
- Click on to save the data entered.

The selected user rights are valid for all users who are in the user groups with the edited user role.

The **User status** is set in the **User list**:

1 Activating a user

- Select a user and open the properties by clicking on under **User management** ▶ **User list**.
- Select **General** in the properties of the user.
- The **active** function is automatically activated under **User status**.

The status of the user is set to **Active** in the user list.

2 Disabling a user

- Deactivate the **active** function by clicking on the check box under **User status**.
- Save the changed settings in the properties by clicking on .

The entry of the user in the user list is grayed out and the status is set to **Deactivated**.

See also

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Data permissions – Definition (chapter 4.5.9, page 105)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

User groups – Properties (chapter 4.5.6.2, page 82)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.5.4 User login

Information on the user management and the settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The user is given a password by the administrator for first-time login by means of the **user management (OMNIS)**. Following first-time login with the password defined by the administrator and change to one's own password, the user can log into the OMNIS Software.

The following steps must be carried out each time you log in to the OMNIS Software:

1 Starting the OMNIS Software and entering the login data

- Start the OMNIS Software.
- In the **Log in to OMNIS Software** dialog, enter the **User ID** and the **Password**.

Passwords of Active Directory users must be changed directly via the Active Directory.
More information on password administration: *(see "Managing the password", chapter 4.5.8, page 102)*

2 Confirming entries

- Click on **[Login]** to confirm the entries.

The user is now logged into the OMNIS Software. The user name of the currently logged-in user is displayed next to the icon.

The maximum number of login attempts can be defined in **User management** ▶ **User management settings** ▶ **Security settings**.

At the time of the first-time login, the user must define his or her future password in the **Change password** dialog which appears automatically. If the **Request change of password** check box has been enabled in the user's properties, this dialog will also appear the next time the user logs in to the OMNIS Software.

If the **Password required** check box has been disabled in **Security settings** ▶ **User management settings** ▶ **User management**, then the user can log into the OMNIS Software without entering his or her password.

Whether or not a password is required for the login is defined by the administrator in **User management** ▶ **User management settings** ▶ **Security settings**. The settings made apply for both types of user management.

If compliance is locked in **Settings** ▶ **Advanced settings**, the **Password required** check box can no longer be disabled.

If the **Audit Trail** function in the **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** option is enabled, then all of the changes made in the OMNIS Software will be recorded and listed in the Audit Trail. Changes which are undertaken directly in the Active Directory are not recorded in the Audit Trail. For more information regarding the recording of entries in the Audit Trail, see: *(see "Audit Trail – Directory", chapter 5.14.5, page 1177)*

See also

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

Locking compliance (chapter 4.3, page 39)

Locking or unlocking the OMNIS Software (chapter 5.4, page 188)

Managing the password (chapter 4.5.8, page 102)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

User groups – Definition (chapter 4.5.6.1, page 81)

User list – Definition (chapter 4.5.5.1, page 70)

User management settings – Subsection (chapter 4.5.4, page 66)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

4.5.6 User groups – Subsection

The following functions are available in **User management** ▶ **User groups**:

-

  Use **Create user group** to create a new user group to which users can be assigned.
-

  Use **Create report** to create a report for the selected user group. The report can be saved as a PDF file or printed out.
-

  Use **Save** to save all changes.
-

  Use **Update view** to update the list of the user groups. All entries are reloaded.
-

  Use **Delete user group** to delete the user group from the database.
-

  The properties of the selected element are displayed in the **Properties** window.

Overview list

The following information is displayed in the overview list:

Name	Name of user group.
Active Directory group	Name of the assigned Active Directory group. **Note:** This column is available only for the use of user management with Active Directory integration and after completed synchronization.
Number of members	Number of active and inactive members.
Created	Date and time the user group was created.

See also

Data permissions – Definition (chapter 4.5.9, page 105)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

User groups – Properties (chapter 4.5.6.2, page 82)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User management – Definition (chapter 4.5.1, page 44)

4.5.6.1 User groups – Definition

Several users are grouped together in a user group. This grouping is used to provide a structured organization of the users.

The following actions can be triggered in **User management** ▶ **User groups**, depending on the type of user management that is activated:

New user groups can be created, existing user groups can be edited, user groups can be deleted and user roles can be assigned to user groups in the **user management (OMNIS)**. Optionally, data permissions can be assigned to the user groups.

The same actions can be triggered in the **User management with Active Directory integration** as in the user management (OMNIS). In addition, the mapping of Active Directory groups to the user groups takes place under the Properties. Optionally, data permissions can be assigned to the user groups.

Information on the central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

See also

Data permissions – Definition (chapter 4.5.9, page 105)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Directory (chapter 4.5.6.3, page 84)

User groups – Properties (chapter 4.5.6.2, page 82)

User groups – Subsection (chapter 4.5.6, page 80)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.6.2 User groups – Properties

Clicking on under **User management** ▶ **User groups** opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 3 subsections **General**, **User roles** and **Data permissions**:

General

The following functions are available for the user group in this subsection:

Name of user group	Entry of the desired name for the user group. The selected name can only be given once.
Comment	Entry of comments about the user group. A maximum of 255 characters are allowed in the comment field.

Additionally, the **mapping** is carried out by the administrator in this subsection if the user management with Active Directory integration is used. The assignment of the selected user group to an existing Active Directory group takes place at the time of the input of the **Distinguished Name**. One Active Directory group can be assigned to multiple user groups in this connection.

The **Distinguished Name** leads to a synchronization group in the Active Directory. This synchronization group must contain all Active Directory groups that will have access to the OMNIS Software. Once the **Distinguished Name** is entered, it is validated.

The **Distinguished Name** must be entered in the correct format. It is not until after completed validation that the **Distinguished Name** leads to a selected Active Directory group.

The **mapping** must take place immediately after the setting up of user management with Active Directory integration and after a restart of the OMNIS Software. In the **OMNIS Client/Server system**, the administrator can log into the OMNIS Software directly without restarting in the last dialog of the setup and carry out the **mapping**. Additional information on central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

User roles

User roles can be assigned to the user group in this subsection. Every user group must be assigned at least one user role.

A user group can also be saved without user roles. In this case, however, the user receives none of the user rights required for being able to work with data in the OMNIS Software.

In addition to the user-defined user roles which can be created in the **User roles** subsection, a number of predefined roles also appear here.

In the event of user management with Active Directory integration, not only are the user groups assigned at the time of the **mapping**, but also the user role and the permissions are assigned to an Active Directory user. Multiple user roles can also be assigned to the same Active Directory user.

The user rights must be assigned to a user role and a user role must be assigned to a user group in the OMNIS Software.

Not until after the synchronization of the OMNIS Software with Active Directory is the Active Directory user given the necessary user rights to permit him or her to work in the OMNIS Software. Without completed synchronization, the Active Directory user can indeed log in, but will not yet see any data in the OMNIS Software.

Additional information regarding the predefined user roles: *(see "User roles – Directory", chapter 4.5.7.3, page 88)*

Data permissions

Data permissions can be assigned to the user group in this subsection.

⊕	**Automatically assigned on create** Data permissions that are automatically added to the data that users from this user group create.
👁	**Data permissions** Data with corresponding data permissions that are visible to users in this user group.

In order for users to be able to see data they have created themselves, they must be assigned at least one data permission for which both **Automatically assigned on create** and **Data permissions** are enabled.

The automatic assignment of data permissions at the time of creation does not involve inherited data permissions.

See also

Assigning data permissions (chapter 4.5.9.2, page 112)

Data permissions – Definition (chapter 4.5.9, page 105)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.6.3 User groups – Directory

Information on the central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The following user groups are available predefined in the OMNIS Software:

- **Administrators**: The first user created is automatically assigned to this user group. As default, this user group has the **Administrator** user role.
- **Instrument managers**: As default, this user group has the **Instrument manager** user role.
- **Laboratory managers**: As default, this user group has the **Lab manager** user role.
- **Method developers**: As default, this user group has the **Method developer** user role.
- **Routine users**: As default, this user group has the **Routine user** user role. If a new user is created, then the **Routine user** user group will be automatically assigned to that person. This assignment can be changed.

For the configuration of the **3rd Party Data Integration API,** Metrohm recommends creating a self-defined user group for API access (e.g. Technical Users). This user group should be assigned a self-defined user role (e.g. Technical User), which is granted all rights for API access.

See also

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Data permissions – Definition (chapter 4.5.9, page 105)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Properties (chapter 4.5.6.2, page 82)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.7 User roles – Subsection

The following functions are available in **User management** ▶ **User roles**:

-
  Use **Create user role** to create a new user role that can be assigned to a user group.
-
  Use **Create report** to create a report for the selected user role. The report can be saved as a PDF file or printed out.
-
  Use **Save** to save all changes.
-
  Use **Update view** to update the list of the user roles. All entries are reloaded.

-

  Use **Delete user role** to delete the user group from the database.
-

  The properties of the selected element are displayed in the **Properties** window.

Overview list

The following information is displayed in the overview list:

Name	Name of the user role.
Number of members	Number of active and inactive members.
Created	Date and time the user role was created.

See also

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.7.1 User roles – Definition

A user role groups together a number of individual rights in the OMNIS Software. User roles are used to make it easier to manage user rights.

Information on the central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

See also

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

User groups – Properties (chapter 4.5.6.2, page 82)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

User roles – Subsection (chapter 4.5.7, page 85)

4.5.7.2 User roles – Properties

Information on the central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Clicking on under **User management** ▶ **User roles** opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 2 subsections **General** and **User rights**:

General

The following functions are available for the user role in this subsection:

Name of the user role	Entry of the desired name for the user role. The selected name must be unique.
Comment	Enter comments about the user group. A maximum of 255 characters are allowed in the comment field.

User rights

Predefined rights can be assigned to the user role in this subsection. In order to work in the OMNIS Software with data, at least one right must be assigned to each user role. By assigning the user role to a user group, all users in the group are equipped with the selected rights.

See also

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

User groups – Properties (chapter 4.5.6.2, page 82)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Directory (chapter 4.5.7.3, page 88)

4.5.7.3 User roles – Directory

Information on the central user management in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The following user roles are available predefined in the OMNIS Software:

- **Administrator**: The Administrator user role includes all the necessary rights for managing the OMNIS Software and users as well as for access to the Audit Trail.
- **Service engineer**: The Service engineer user role cannot be assigned to any user group and is provided exclusively for work by the regional Metrohm service representative. The trained and certified regional Metrohm service representative can log in to the OMNIS Software using a dongle to carry out service work.
- **Instrument manager**: The Instrument manager user role includes all the necessary rights for maintenance of laboratory devices and accessories.
- **Laboratory managers**: The Laboratory manager user role includes access to the **Samples** and **Audit Trail** work areas as well as all rights for the **Processes**, **Equipment** and **Models** work areas.
- **Method developer**: The Method developer user role includes access to the **Samples** and **Processes** work areas as well as all rights for the **Equipment** and **Models** work areas.
- **Support engineer**: The Support engineer user role includes all the rights that are available in the OMNIS Software. In case of technical problems, the trained and certified Metrohm support can login to the OMNIS Software using a dongle to provide professional support. This user role is a completely internal functionality that is only provided for the work of Metrohm support. The Support engineer user role cannot be assigned to any user group.
- **Routine users**: The Routine user user role includes all the necessary rights for daily work in the laboratory.

For the configuration of the **3rd Party Data Integration API,** Metrohm recommends creating a self-defined user role for API access (e.g. Technical User). This user role must be assigned all rights that are available for API access. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

The user role should only be created for technical purposes to enable secure communication between the OMNIS Software and the third-party software. Technical users are user entries that are not assigned to a real person.

See also

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Data permissions – Definition (chapter 4.5.9, page 105)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Directory (chapter 4.5.6.3, page 84)

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User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.7.4 User rights – Directory

Rights can be assigned to the user roles in **User management** ▶ **User roles** ▶ **Properties** ▶ **User rights**. These rights affect what the users with this user role can view and execute in the OMNIS Software.

The right can be activated or deactivated by clicking on the respective check box.

Certain rights can be used only if the corresponding work area is visible or if a higher-level right is also activated. Attention must be paid to dependencies.

Changed rights will not take effect until after a restart of the OMNIS Software.

New rights are automatically assigned to a user role only for new installations starting with OMNIS Software version 3.0.0. Otherwise new rights are not automatically assigned to a user role but must be added to it manually instead. Contact the internal IT administrator in the event of missing rights.

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

By assigning the user role to a user group, all users in the group are equipped with the selected rights:

Samples	Permission for the following actions
Manage samples	This right permits general access to the samples work area. Additional differentiated lower-level rights can be assigned for managing or executing samples or subsamples. As soon as a lower-level right is enabled, the **Manage samples** and **Manage sample lists** rights are automatically also assigned.
Manage sample lists	This right permits access to the Sample lists subsection. As soon as a lower-level right is enabled, the **Manage sample lists** right is automatically also assigned.
Create and duplicate sample lists	▪ Open sample lists, rename and save them. ▪ Create and duplicate sample lists. ▪ Create a new sample list with selected samples and subsamples.
Remove sample lists from the local client	▪ Remove local sample lists. **Note**: Applicable only in the **OMNIS Client/Server system**.
Delete sample lists	▪ Delete sample lists (contained samples and subsamples are not deleted).

Samples	Permission for the following actions
Add samples/ subsamples	▪ Open sample lists, rename and save them. ▪ Add samples and subsamples to a sample list. ▪ Copy samples and subsamples from a sample list. ▪ Select a sample profile. ▪ The **Edit samples/not analyzed subsamples** right is also required to edit the sample data and subsample data.
Add sample data	▪ Add sample data in the sample list.
Edit samples/not analyzed subsamples	▪ Open sample lists, rename and save them. ▪ Edit sample data and subsample data from subsamples that have not been analyzed.
Remove, cut and paste samples/ subsamples	▪ Open sample lists, rename and save them. ▪ Remove samples and subsamples from a sample list. ▪ Cut samples and subsamples from a sample list. ▪ Paste samples and subsamples from a sample list.
Delete samples/subsamples	▪ Open sample lists, rename and save them. ▪ Delete selected samples and subsamples permanently from the sample list or search query (the samples and subsamples can have any status when deleting).
Import samples	▪ Open sample lists, rename and save them. ▪ Import CSV files and OSIN files manually.
Export samples	▪ Open sample lists, rename and save them. ▪ Export samples, associated subsamples and determination data. ▪ The **Manage search queries** right is also required to export samples, associated subsamples and determination data from the search queries.
Lock samples	▪ Open sample lists, rename and save them. ▪ Lock the samples. Changes to sample data and the adding and deletion of subsamples are prevented. ▪ Unlock the samples. ▪ Read-only view of the sample data (subsample data is not read-only when samples are locked).

Samples	Permission for the following actions
Start determinations with unreleased operating procedures	▪ Open sample lists, rename and save them. ▪ Start the determinations. ▪ Select the type of the determinations. **Note**: In **OMNIS Stand-Alone**: **Unreleased operating procedures** are operating procedures without Level 2 signature. In the **OMNIS Client/Server system**: **Unreleased operating procedures** are operating procedures that have a status other than **published**.
Start determinations with released operating procedures	▪ Open sample lists, rename and save them. ▪ Start or stop determinations. ▪ Select the type of the determinations. **Note**: In the **OMNIS Stand-Alone**: **Released operating procedures** are operating procedures with Level 2 signature. In the **OMNIS Client/Server system** without activated conformity: **Released operating procedures** are operating procedures that have the status **published**. In the **OMNIS Client/Server system** with enabled conformity: **Released operating procedures** are operating procedures that have the status **published** and Level 2 signature.
Start determinations with expired equipment	▪ Start the determination with expired equipment.
Skip running command	▪ Skip an ongoing command in the **Live data** subsection during a determination.
Reprocess subsamples	▪ Change the evaluation of the analysis. ▪ Recalculate results. ▪ Modify the subsample data after the analysis. This leads to the recalculation of results. ▪ Do not take results in statistics into account anymore. ▪ Reevaluate and correct predictions.
Archive samples	▪ Archive the samples. **Note**: In the **OMNIS Client/Server system**: Remove sample lists from the local OMNIS Client.

Samples	Permission for the following actions
Reset subsamples to status "Ready"	▪ Reset the subsamples to the "Ready" status.
Create reports manually	▪ Create reports.
Manage control charts	▪ Display the Control charts subsection. ▪ Open control charts. ▪ Create, edit, save and delete control charts.
Display control charts	▪ Display the Control charts subsection. ▪ Open control charts.
Manage search queries	▪ Create, edit, rename, save and delete search queries. **Note**: In the **OMNIS Client/Server system**: Create, edit, rename, save and delete server search queries. ▪ The **Export samples** right is also required to export samples, associated subsamples and determination data from the search queries. ▪ The **Create and duplicate sample lists** right is also required to save the search query as a new sample list.
Manage sample profiles	The right permits general access to the Sample profiles and Server sample profiles subsections. Additional differentiated lower-level rights can be assigned for managing or executing sample profiles or server sample profiles. As soon as a lower-level right is enabled, the **Manage sample profiles** right is automatically also assigned.
Manage sample profiles and server sample profiles	▪ Display sample profiles subsection. ▪ Open sample profiles. ▪ Create, edit, save and delete sample profiles. **Note**: Applicable in **OMNIS Stand-Alone** and **OMNIS Client/Server system**. ▪ Display server sample profiles subsection. ▪ Download server sample profiles. **Note**: Applicable only in the **OMNIS Client/Server system**.

Samples	Permission for the following actions
Publish sample profiles	▪ Publish sample profiles. **Note**: Applicable only in the **OMNIS Client/Server system**.
Delete server sample profiles	▪ Delete server sample profiles. **Note**: Applicable only in the **OMNIS Client/Server system**.
Manage system variables	This right permits access to the System variables subsection. As soon as a lower-level right is enabled, the **Manage system variables** right is automatically also assigned.
Create and edit system variables	▪ Create, edit and save system variables.
Delete system variables	▪ Delete system variables.
Sign subsamples (level 1)	▪ Sign subsamples on Level 1. ▪ Delete Level 1 signatures for subsamples.
Sign subsamples (level 2)	▪ Sign subsamples on Level 2. ▪ Delete Level 2 signatures for subsamples.
Delete subsamples signatures	▪ Delete Level 1 or Level 2 signatures for subsamples.

Processes	Permission for the following actions
Manage processes	This right permits general access to the process work area. Additional differentiated lower-level rights can be assigned for managing or executing operating procedures or methods. As soon as a lower-level right is enabled, the **Manage processes** right is automatically also assigned.

Processes	Permission for the following actions
Manage operating procedures/methods	▪ Display operating procedures and methods subsections. ▪ Create, open, edit, save, duplicate, import and export operating procedures and methods. ▪ Restore operating procedures and methods from analyzed subsamples. **Note**: Applicable in **OMNIS Stand-Alone** and **OMNIS Client/Server system**. ▪ Display server operating procedures and server methods subsections. ▪ Download server operating procedures and server methods. **Note**: Applicable only in the **OMNIS Client/Server system**.
Delete operating procedures/methods	Delete operating procedures and methods. **Note**: Only applicable in **OMNIS Stand-Alone**.
Manage operating procedures/methods (advanced)	In order to use this right and the lower-level rights, the **Manage operating procedures/methods** right is also required. As soon as a lower-level right is enabled, the **Manage operating procedures/methods (advanced)** and **Manage processes** rights are automatically also assigned. **Note**: Applicable only in the **OMNIS Client/Server system**.
Publish operating procedures/methods	▪ Publish operating procedures and methods. **Note**: Applicable only in the **OMNIS Client/Server system**.
Withdraw operating procedures/methods	▪ Withdraw operating procedures and methods. **Note**: Applicable only in the **OMNIS Client/Server system**.
Delete server operating procedures/server methods	▪ Delete server operating procedures and server methods. **Note**: Applicable only in the **OMNIS Client/Server system**.

Processes	Permission for the following actions
Remove local operating procedures/ methods	▪ Remove local operating procedures and methods. **Note**: Applicable only in the **OMNIS Client/Server system**.
Sign operating procedures/methods (level 1)	▪ Sign operating procedures and methods on Level 1. ▪ Delete all Level 1 signatures with operating procedures or methods.
Sign operating procedures/methods (level 2)	▪ Sign operating procedures and methods on Level 2. ▪ Delete all Level 2 signatures with operating procedures or methods.
Delete operating procedures or methods signatures	▪ Delete all Level 1 or Level 2 signatures with operating procedures or methods.

Equipment	Permission for the following actions
Manage equipment	The right permits general access to the equipment. Additional differentiated lower-level rights can be assigned for managing instruments and other equipment. As soon as a lower-level right is enabled, the **Manage equipment** right will also be assigned automatically.
Manage instruments	This right permits access to the Instruments subsection. As soon as a lower-level right is enabled, the **Manage instruments** right is automatically also assigned.
Edit instruments	▪ Add instruments manually. ▪ Reserve and release instruments. ▪ Edit instrument properties.
Remove instruments	▪ Remove the instruments. ▪ Remove the instruments and functional units.
Manage manual control	This right permits access to the manual control of instruments and functional units. As soon as a lower-level right is enabled, the **Manage manual control** right will also be assigned automatically.

Equipment	Permission for the following actions
Operate instruments	▪ Display instruments. ▪ Execute functions of instruments and functional units.
Assign lift heights	▪ Assign the current lift height to a predefined lift height. ▪ Display of the **Assign current height** button.
Manage work systems	This right permits access to the Work systems subsection. As soon as a lower-level right is enabled, the **Manage work systems** right is automatically also assigned.
Edit work systems	▪ Create, edit and save work systems.
Operate work systems	▪ Open and stop the work system.
Delete work systems	▪ Delete the work systems.
Manage sensors	This right permits access to the Sensors subsection. As soon as a lower-level right is enabled, the **Manage sensors** right is automatically also assigned.
Edit sensors	▪ Add and save the sensor. ▪ Edit the properties of the sensor. ▪ Define the advance warning time.
Remove sensors	▪ Delete the sensor.
Manage solutions	This right permits access to the Solutions subsection. As soon as a lower-level right is enabled, the **Manage solutions** right is automatically also assigned.
Edit solutions	▪ Add and save the solution. ▪ Edit the properties of the solution. ▪ Define the advance warning time.
Remove solutions	▪ Delete the solutions.
Manage calibration buffers	▪ Create, edit, save and delete tables of calibration buffers. ▪ Delete calibration buffers.
Manage standards	This right permits access to the Standards subsection. As soon as a lower-level right is enabled, the **Manage standards** right is automatically also assigned.

Equipment	Permission for the following actions
Edit standards	▪ Import standards. ▪ Edit the properties of the standard.
Delete standards	▪ Delete standards.
Manage sample racks	This right permits access to the Sample racks subsection. As soon as a lower-level right is enabled, the **Manage sample racks** right will also be assigned automatically.
Edit sample racks	▪ Save and import sample racks. ▪ Edit the properties of the sample rack.
Delete sample racks	▪ Delete the sample racks.

In order to be able to create and edit models, the respective license is required in addition to the user rights listed below.

Models	Permission for the following actions
Manage models	This right permits general access to the Models work area. Additional differentiated lower-level rights for models, model hierarchies or slope/y-intercept corrections can be assigned. As soon as a lower-level right is enabled, the permission for the **Manage models** right is automatically enabled as well.
Manage quantification models	This right permits access to the Quantification models subsection. As soon as a lower-level right is enabled, the **Manage quantification models** right is automatically also assigned.
Edit quantification models	▪ Create, open, edit, save, publish and duplicate quantification models. ▪ Import and export quantification models.
Delete quantification models	▪ Delete quantification models.
Manage slope/y-intercept corrections	This right permits access to the Slope/y-intercept correction subsection. As soon as a lower-level right is enabled, the **Manage slope/y-intercept corrections** right is automatically also assigned.

Models	Permission for the following actions
Edit slope/y-intercept corrections	▪ Create, save and publish slope/y-intercept corrections. ▪ Import and export slope/y-intercept corrections.
Delete slope/y-intercept corrections	▪ Delete slope/y-intercept corrections.
Manage identification models	This right permits access to the Identification models subsection. As soon as a lower-level right is enabled, the **Manage identification models** right is automatically also assigned.
Edit identification models	▪ Create, open, edit, save, publish and duplicate identification models. ▪ Import and export identification models.
Delete identification models	▪ Delete identification models.
Manage model hierarchies	This right permits access to the Model hierarchies subsection. As soon as a lower-level right is enabled, the **Manage model hierarchies** right is automatically also assigned.
Edit model hierarchies	▪ Create, open, edit, save and publish model hierarchies. ▪ Import and export model hierarchies.
Delete model hierarchies	▪ Delete model hierarchies.

Audit Trail	Permission for the following actions
Show Audit Trail	▪ Display Audit Trail subsection. ▪ Filter Audit Trail and check for integrity.
Export Audit Trail	▪ Export the Audit Trail in a CSV file.
Archive Audit Trail	▪ Archive Audit Trail. **Note**: Applicable only in **OMNIS Stand-Alone**.

User management	Permission for the following actions
Manage user settings/lists and groups	This right permits access to the following subsections: ▪ Display the following subsections: – User management settings – User list – User groups – User roles As soon as a lower-level right is enabled, the **Manage user settings/lists and groups** right is automatically also assigned
Edit user settings/lists and groups	▪ Create, edit and disable or enable users. ▪ Create, edit, save and delete user groups. ▪ Create, edit, save and delete user roles. ▪ Edit log in behavior and lock behavior. ▪ Edit password guidelines.
Delete user groups	▪ Delete user groups.
Manage data permissions	This right permits access to the Data permissions subsection. As soon as a lower-level right is enabled, the **Manage data permissions** right is automatically also assigned.
Edit data permissions	▪ Set up and enable or disable data permissions. Block deactivation of data permissions. ▪ Display the User groups subsection with restrictions with access to the **Data permissions** subsection in the **Properties** window. ▪ Assign existing data permissions to the user groups.
Delete data permissions	▪ Delete existing data permissions of the user groups.
Assign data permissions	▪ Assign existing data permissions to the data.
Log in and filter data despite missing assignment of data permissions	▪ Log in to the OMNIS Software after blocking and despite missing data permission assignments. ▪ Filter data after activation and despite missing data permission assignments. (Filter of data permissions can be used in the title bar) ▪ Filter data after blocking. (Filter of data permissions can be used in the title bar)

User management	Permission for the following actions
Manage user roles	This right permits access to the User roles subsection. As soon as a lower-level right is enabled, the **Manage user roles** right is automatically also assigned.
Edit user roles	▪ Create, edit and save user roles.
Delete user roles	▪ Delete user roles.

Settings	Permission for the following actions
Manage settings	This right permits general access to the Settings work area. Additional differentiated lower-level rights can be assigned. As soon as a lower-level right is enabled, the **Manage settings** right is automatically also enabled.
Manage general settings	▪ Edit all general settings (dialog languages, emergency stop function, preliminary run test). ▪ Edit print settings. ▪ Edit notifications. **Note**: In the **OMNIS Client/Server system**, the settings apply only for the individual OMNIS Client.
Manage advanced settings	▪ Edit all advanced settings (system languages). ▪ Activate user management. ▪ Edit the conformity settings. **Note**: In the **OMNIS Client/Server system**, the settings apply for all the connected OMNIS Clients.
Activate software licenses	▪ Add software licenses.
Manage database settings	▪ Display the Database settings subsection. ▪ Display occupied and free space in the database. ▪ View connection settings of the external database.
Database backup	▪ Back up the local database manually and automatically.
Change operation mode	▪ Change the operation mode for the database configuration in the OMNIS Software to perform service activities.

API access	Permission for the following actions
Retrieve dataset	▪ Read samples, subsamples, sample lists, sample profiles and operating procedures via a web API (interface). **Note**: For this right, the web API must be set up and the necessary software license must be enabled.
Create and update dataset	▪ Create and update samples, subsamples and sample lists via a web API. **Note**: For this right, the web API must be set up and the necessary software license must be enabled.
Start or stop determinations	▪ Use a web API to start or stop determinations of selected subsamples. **Note**: For this right, the web API must be set up and the necessary software license must be enabled. In addition, at least one of the existing user rights must be enabled to be able to start determinations.

See also

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Data permissions – Definition (chapter 4.5.9, page 105)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Properties (chapter 4.5.6.2, page 82)

User list – Definition (chapter 4.5.5.1, page 70)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

4.5.8 Managing the password

Information on the central management of the security settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

All users can modify their own passwords at any time by using the **user management (OMNIS)**:

1 Replacing the current password

- Click on in the title bar of the OMNIS Software.
- Select **[Change password]** in the selection list to replace the current password with a new one.

2 Changing the password

- Enter a new password in the **Change password** dialog and confirm by entering it again.
- Save the new password by clicking on **[Change password]**.

If the **Password required** check box has been deactivated in **User management** ▶ **User management settings** ▶ **Security settings**, then the user can log into the OMNIS Software without entering his or her password.

Whether or not a password is required for the login is defined by the administrator in **User management** ▶ **User management settings** ▶ **Security settings**. The settings made apply for both types of user management.

If compliance is locked in **Settings** ▶ **Advanced settings**, the **Password required** check box can no longer be disabled.

If the **Password never expires** check box was enabled in the properties of a user under **User management** ▶ **User list**, the user's password never expires, even if an expiry time for the password has been defined in **Security settings**.

Active Directory users do not have the possibility of changing their passwords in the OMNIS Software. In the event of active Active Directory integration, only the administrator with which the Active Directory integration was carried out can change his or her password in the OMNIS Software. Passwords of Active Directory users are only changed and managed via the Active Directory.

If users in specific roles forgot their passwords or if the maximum number of login attempts has been exceeded, then the following steps must be carried out:

Password forgotten

1 Users of the OMNIS Software

- Users must consult the administrator for resetting their password. The administrator defines a new password for the user, which he can replace with his own password at the next login.

If the **Request change of password** check box has been enabled in the properties of the user under **User management ▶ User list**, the user will not receive a new password from the administrator for the change of password. The user himself must define and confirm his new password in the **Change password** dialog the next time he logs in.

2 Active Directory users

- Active Directory users must consult the internal IT administrator for resetting their password.

3 Administrator with which the Active Directory integration was carried out

- The administrator cannot reset the password on his own.
- If the administrator has previously furnished one or more Active Directory users with the **Manage users** right, then the administrator can consult these users. These Active Directory users have administrator rights because of the distribution of rights and can in this case reset the password of the administrator. The administrator also has the option of contacting the regional Metrohm representative.

Metrohm recommends defining at least one Active Directory user as an additional administrator in the OMNIS Software.

If the **Audit Trail** function in the **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** option is activated, then all of the changes made in the OMNIS Software will be recorded and listed in the Audit Trail. Changes which are undertaken directly in the Active Directory are not recorded in the Audit Trail. For more information regarding the recording of entries in the Audit Trail, see: *(see "Audit Trail – Directory", chapter 5.14.5, page 1177)*

See also

Data exchange with third-party software – Definition (chapter 4.9, page 147)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

Locking compliance (chapter 4.3, page 39)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User list – Definition (chapter 4.5.5.1, page 70)

User list – Properties (chapter 4.5.5.2, page 72)

User management settings – Subsection (chapter 4.5.4, page 66)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Definition (chapter 4.5.7.1, page 86)

4.5.9 Data permissions – Definition

Data permissions are used to define which data specific users can see and edit in the OMNIS Software. Data permissions are assigned to specific data (e.g. operating procedures or methods) and specific user groups. Users have access only to data that they need to carry out their work in the areas of the OMNIS Software that are enabled for them by user rights. This minimizes sources of error and reduces processing times.

The data permissions are set up and managed by the user who has the **Manage data permissions** user right under **User management ▶ Data permissions**.

Users are assigned their data permissions via the user group in which they are located under **User management ▶ User groups**. The more data permissions assigned to a user, the more data will be enabled for that user to view. This assignment can be made only by a user who has the **Assign data permissions** user right.

Metrohm recommends creating a self-defined user group (e.g. data permission manager) for the configuration of data permissions. This user group should be assigned a self-defined user role (e.g. data permission manager), which is granted all user rights for the management and assignment of data permissions.

Metrohm recommends also assigning the **Log in and filter data despite missing assignment of data permissions** user right to the data permission manager. This ensures that the data permissions manager can always log in to the OMNIS Software and make any missing data permission assignments.

Additional information on user rights for data permissions: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

Example configuration that can be used for orientation when implementing the data permission: *Data permissions – Technical White Paper*

Requirements for the use of data permissions:

- **User management:** The use of the data permissions requires an enabled user management.

- **User rights:** To be able to manage and assign data permissions, you will need your own user rights.

When using data permissions, the following rules apply in the Samples work area:

- In the following cases, the data permissions are assigned to the data with **Automatically assigned on create** of the currently logged in user:
  - When creating sample lists, samples or sample profiles.
  - When inserting copied samples or partial samples.
  - When duplicating sample lists, samples or sample profiles.
  - When importing samples or sample profiles.
  - When restoring operating procedures and associated methods from subsamples.
  - When downloading sample profiles.
    Note: Applicable only in the **OMNIS Client/Server system**.
  - When publishing sample profiles, the data permissions of the user currently logged in are assigned, but can still be edited. Any data permissions can be removed when publishing. At least one data permission must be assigned to access the sample profiles.
    If the sample profile contains a data permission and this is to be displayed to another user group with different data permissions, then the sample profile must be published once again.
    Sample profiles containing a withdrawn operating procedure or method cannot be republished.
    Note: Applicable only in the **OMNIS Client/Server system**.
- After the adding of subsamples and the subsequent selection of the operating procedure in the sample list, the data permissions of the operating procedure are then added to the subsample. The data permissions of the subsample are added to the sample.
- When a subsample is deleted, the data permissions that the sample previously received from the subsample are not removed from the sample.
- Changes in the data permissions of an operating procedure have the following effect on the subsamples to which this operating procedure is assigned:
  - Changes to the data permissions of an operating procedure that is assigned to analyzed subsamples do not result in changes to the data permissions for the subsamples that have already been analyzed.
  - Changes to the data permissions of an operating procedure that is assigned to subsamples in the **Ready** status are synchronized.

When using data permissions, the following rules apply in the Processes work area:

- In the following cases, the data permissions are assigned to the data with **Automatically assigned on create** of the currently logged in user:
  - When importing operating procedures or methods.
  - When duplicating operating procedures or methods.
  - When publishing operating procedures or methods, the data permissions of the user currently logged in are assigned, but can still be edited. Any data permissions can be removed when publishing. At least one data permission must be assigned to access the operating procedures or methods. If the operating procedure or method contains data permissions and these are to be displayed to another user group with different data permissions, then the operating procedure or method must be published once again.
    Withdrawn operating procedures, methods or operating procedures containing withdrawn methods cannot be republished.
    Note: Applicable only in the **OMNIS Client/Server system**.
- When importing operating procedures or methods that already exist in the database but do not have the data permissions of the currently logged in user, the **[Overwrite]** option will not be visible.

When using data permissions, the following rules apply in the Models work area:

- With the **Update methods** function, only methods with the data permissions of the currently logged in user are updated when publishing models if data permission filtering is enabled.

When using data permissions, the following rules apply in the User management work area:

- In order for users to be able to see data they have created themselves, they must be assigned at least one data permission for which both **Automatically assigned on create** and the **Data permissions** are enabled.
- A maximum of 2,000 data permissions can be created.
- A maximum of 100 data permissions can be assigned to a user. If the user is assigned to several user groups, then the data permissions of the user groups will be assigned to the user.
- Data permissions can be created and deleted only with an existing connection to the OMNIS Server.
  Note: Applicable only in the **OMNIS Client/Server system**.
- Changes to the settings for data permissions (enable, disable, block) are applied to other OMNIS Clients only after the OMNIS Software has been restarted.
  Note: Applicable only in the **OMNIS Client/Server system**.

See also

Assigning data permissions (chapter 4.5.9.2, page 112)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

Filtering data permissions (chapter 4.5.9.3, page 115)

Managing data permissions (chapter 4.5.9.1, page 108)

Managing users (chapter 4.5.5.3, page 74)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Tags – Definition (chapter 5.9, page 203)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Properties (chapter 4.5.6.2, page 82)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

4.5.9.1 Managing data permissions

In the **OMNIS Client/Server system**, changes to the settings for data permissions (enable, disable, block) are not applied to other OMNIS Clients until after the OMNIS Software has been restarted.
Additional information on data permissions: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

The data permissions are managed under **User management ▶ Data permissions**. Management includes setting up and enabling or disabling data permissions. In addition, the deactivation of the data permissions can be locked:

- *Setting up data permissions*: This allows user-defined data permissions to be created and set up. Additional data permissions can be added at any time.
- *Activation/deactivation of data permissions*: This allows the defined data permissions to be activated for the entire OMNIS Software. It is possible to disable the data permissions once again. If data permissions are activated, users can use a filter to decide for themselves whether they only want to see the data assigned to them or all available data.
- *Block deactivation of data permissions*: This means that the activated data permissions cannot be deactivated again. The blocking of the deactivation can no longer be reversed.

Setting up the data permissions

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- User management is enabled.
- The connection to the OMNIS Server is available in the **OMNIS Client/Server system**.

1 Entering data permissions

- Enter a name for a new data permission under **User management** ▶ **Data permissions** ▶ **Setup** in the **[Enter name]** input field.
- Confirm the entry by clicking on **+** or **[Enter]**.

Pay attention to the following when creating data permissions:
- All punctuation marks and numbers are permitted.
- The same data permission cannot be assigned more than once, even if the use of upper and or lower case differs.
- A maximum of 2,000 data permissions can be created.

After validation, the data permission is saved in the database and displayed in the list. Subsequently, it can be assigned to the desired user groups and data (e.g. operating procedures or methods).

2 Deleting data permissions

- Click on ✕ to delete individual data permissions.
- Confirm the dialog by clicking on **[Delete]**.

The data permission is permanently deleted from the database.

This dialog appears only if a data permission has already been assigned to user groups and data. This deletes both the data permission and the assignments to the user groups and data. The user groups and data are retained.

Activation or deactivation of data permissions

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- User management is enabled.
- The connection to the OMNIS Server is available in the **OMNIS Client/Server system**.
- At least one data permission is set up.
- The data permissions are assigned to the user groups and data: *(see "Assigning data permissions", chapter 4.5.9.2, page 112)*

1 Activating data permissions

- Activate the assigned data permissions by clicking on **[Activate data permissions]**.
- Confirm the dialog by clicking on **[Activate]**.

After activation, users see a filtered view of the data in accordance with their assigned data permissions. The option to switch to an unfiltered view is still available: *(see "Filtering data permissions", chapter 4.5.9.3, page 115)*

As long as blocking has not been activated, the activation of data permissions can be undone. This allows incorrectly assigned data permissions to be corrected in the event of problems without affecting users.

If the data permissions have not yet been activated but user groups and data have already been assigned, then the user's data permissions defined under **Automatically assigned on create** ⊕ are already applied to the newly created data when new data is created.

2 Deactivating data permissions

- Deactivate the assigned data permissions by clicking on **[Deactivate data permissions]**.
- Confirm the dialog by clicking on **[Deactivate]**.

After deactivation, all available data is displayed again for all users.

Data permissions that have already been assigned are not deleted from the database. They are retained so that they can be reactivated if necessary.

Blocking deactivation of data permissions

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- User management is enabled.
- The connection to the OMNIS Server is available in the **OMNIS Client/ Server system**.
- The data permissions are activated.

1 Blocking deactivation of data permissions

- Block the deactivation of the data permissions by clicking on **[Lock data permissions]**.
- Confirm the dialog by clicking on **[Lock]**.

After blocking, users see only the data relevant to them in accordance with their assigned data permissions. The option to switch to an unfiltered view to see all data again is no longer available.

After blocking, the activated data permissions cannot be deactivated again. The blocking of the deactivation cannot be reversed. Additional data permissions can still be created and previously assigned data permissions can be edited even after blocking.

Metrohm recommends assigning the **Log in and filter data despite missing assignment of data permissions** user right to at least one user. This user can always log in to the OMNIS Software, activate or deactivate the data permission filter and make assignments of missing data permission based on the user right.

See also

Assigning data permissions (chapter 4.5.9.2, page 112)

Data permissions – Definition (chapter 4.5.9, page 105)

Filtering data permissions (chapter 4.5.9.3, page 115)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User management – Definition (chapter 4.5.1, page 44)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Directory (chapter 4.5.7.3, page 88)

4.5.9.2 Assigning data permissions

Additional information on data permissions: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

- *Assigning data permissions to user groups*
- *Assign data permissions to data*
- *Remove data permissions from data*

Assigning data permissions to user groups

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The data permissions are set up. Additional information: *(see "Managing data permissions", chapter 4.5.9.1, page 108)*

1 Selecting a user group

- Under **User management** ▶ **User groups**, select a user group to whom data permissions are to be assigned.

2 Opening data permissions

- Click on to open the **Properties** window.
- In the **Properties** window, select the **Data permissions** subsection.

3 Assigning data permissions to the user groups

- Assign the desired **Data permissions** by clicking on the respective check box.

Automatically assigned on create: Data permissions with a check mark under are automatically added to the data that the user creates from this user group.

Data permissions: Data permissions with a check mark under make data visible to the user in this user group. The more data permissions assigned to a user group, the more data will be enabled for its view.

Metrohm recommends setting up the user groups in such a way that each user has at least one data permission for which both **Automatically assigned on create** and **Data permissions** are enabled. This ensures that the user can see their own data. If a missing assignment is detected, users must contact the data permissions manager.

A maximum of 100 data permissions can be assigned to a user. If the user is assigned to several user groups, then the data permissions of the user groups will be assigned to the user.

Assigning data permissions to data

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The data permissions are set up. Additional information: *(see "Managing data permissions", chapter 4.5.9.1, page 108)*

1 Selecting data

- Select the desired data in the following subsections:
  - **Samples** ▶ **Sample lists**
  - **Samples** ▶ **Sample profiles**
  - **Processes** ▶ **Operating procedures**
  - **Processes** ▶ **Methods**

  In the **OMNIS Client/Server system**:
  - **Samples** ▶ **Server sample profiles**
  - **Processes** ▶ **Server operating procedures**
  - **Processes** ▶ **Server methods**

2 Opening an input field

- Double-click to select the desired field in the **Data permissions** column.

An input field below the selected line opens.

The **Data permissions** column is visible only if the user has been assigned the user right **Assign data permissions**.

3 Assigning existing data permissions

- The following options are available for assigning an existing data permission:
  - Double-click in the input field and select the desired data permission from the selection list.
  - Write an existing data permission in the input field and select the desired data permission from the selection list.
  - Click in the input field and press the downwards **[arrow]** key to mark the desired data permission and confirm with another click or with **[Enter]**.

The data permission is displayed in the input field and in the **Data permissions** column.

Removing data permissions from data

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The data permissions are set up. Additional information: *(see "Managing data permissions", chapter 4.5.9.1, page 108)*

1 Selecting data

- Select the desired data in the following subsections:
  - **Samples ▶ Sample lists**
  - **Samples ▶ Sample profiles**
  - **Processes ▶ Operating procedures**
  - **Processes ▶ Methods**

2 Opening an input field

- Double-click to select the desired field in the **Data permissions** column.

An input field below the selected line opens.

3 Removing individual data permissions

- Remove the data permission by clicking on ✕ in the data permission.
- Alternatively, data permissions can also be removed with the **[Backspace]** key.

If the user removes their last data permission of a dataset when data permission filtering is activated, then this data set will no longer be visible in the OMNIS Software.

See also

Data permissions – Definition (chapter 4.5.9, page 105)

Filtering data permissions (chapter 4.5.9.3, page 115)

Managing data permissions (chapter 4.5.9.1, page 108)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Publishing the sample profile (chapter 5.10.5.5, page 267)

4.5.9.3 Filtering data permissions

Additional information on data permissions: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

- *Filter data permissions*
- *View own data permissions*

Filtering data permissions

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The data permissions are set up and enabled. Additional information: *(see "Managing data permissions", chapter 4.5.9.1, page 108)*
- The user is assigned at least one data permission for which both **Automatically assigned on create** and **Data permissions** are enabled.

1 Activating or deactivating filters

- Click on in the title bar of the OMNIS Software.
- In the selection list, activate or deactivate the filter next to **[Data permissions]**.

With , all data is filtered according to the data permissions. The user only sees data that has been assigned data permissions to which they have access.

With , all data is listed unfiltered.

If the deactivation of data permissions is blocked, then the filter can be activated only by users who have been assigned the **Log in and filter data despite missing assignment of data permissions** user right if data permissions are not assigned. This user can always log into the OMNIS Software and filter data based on the user rights.

Viewing own data permissions

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The data permissions are set up and enabled. Additional information: *(see "Managing data permissions", chapter 4.5.9.1, page 108)*
- The user is assigned at least one data permission for which both **Automatically assigned on create** and **Data permissions** are enabled.

1 Viewing own data permissions

- Click on in the title bar of the OMNIS Software.
- Click on **[Own data permissions]** to open the dialog with the data permissions of the user currently logged in.

Automatically assigned on create: Data permissions with a check mark under are automatically added to the data (e.g. operating procedures) that the user currently logged in creates.

Data permissions: If there is a check mark under for data permissions, then the data to which this data permission has been assigned will be visible to the user currently logged in.

See also

Assigning data permissions (chapter 4.5.9.2, page 112)

Data permissions – Definition (chapter 4.5.9, page 105)

Managing data permissions (chapter 4.5.9.1, page 108)

4.6 Database – Definition

The term **Database** in the OMNIS Software refers to a part of the system in which all the data from the OMNIS Software, e.g. determinations, samples or information about assigned instruments, is saved.

All the details regarding the database can be found in the OMNIS Software under **Settings** ► **Database settings** or on the **Overview** tab in the **OMNIS Database Administration** program. If the database size is critical, information regarding the occupied space of the local database is displayed in the title bar of the OMNIS Software.

To perform service activities, a total of 3 operation modes of the OMNIS system must be configured. For this, 3 databases must be prepared and set up for each individual operation mode.

Depending on the installation type (**OMNIS Stand-Alone** or **OMNIS Client/Server system**), you can select either a **local database (Microsoft SQL Server Express)** or a **connection to an external database on a dedicated Microsoft SQL Server** (*Installing the OMNIS Software*) at the time of initial installation of the OMNIS Software.

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

- **OMNIS Stand-Alone with local database:** The local database **Microsoft SQL Server Express** is set up on the computer on initial installation of the OMNIS Software. Microsoft SQL Server Express is a relational database system for the structured storage of data with a maximum size of 10 GB. The database is saved **locally** on the computer and is only used for the locally installed OMNIS Software.

- **OMNIS Stand-Alone with connection to an external database:** A connection to an **external database on a dedicated Microsoft SQL Server** is set up on initial installation of the OMNIS Software. This database first has to be set up on a dedicated Microsoft SQL Server for the OMNIS Software.
  - Setting up the dedicated Microsoft SQL Server and the database is the responsibility of the internal IT administrator of the user. The administrator also defines the size of the database and determines for example automatic backup files for the database. The database is stored on the dedicated server of the user and is available only to users with the necessary access rights.
    Information on the supported versions of the Microsoft SQL Server: *Database server*
    Instructions for preparing the external database for use in the OMNIS Software (**OMNIS Stand-Alone**): *Preparing the database*
  - Even after installation from a local database, it is possible to switch to an external database. The change can be done in the **OMNIS Database Administration** program on the **Overview** tab. It is no longer possible to switch to the **Microsoft SQL Server Express** local database once the external database has been set up.
    Instructions on transferring a local database that is already in use to a dedicated database server: *Transferring the database*

If the connection between the OMNIS Software and the database server is interrupted, then an error message will appear. The OMNIS instruments are stopped automatically. The OMNIS Software needs to be closed and restarted manually to continue working with it.

- **OMNIS Client/Server system:** Each OMNIS Client works with the local database (**Microsoft SQL Server Express)** and synchronizes with the **OMNIS Server** within the **OMNIS Client/Server system**. The OMNIS Server works with an external database on which all the generated data is stored centrally. This data is available to all connected OMNIS Clients. The central database first has to be set up on a dedicated Microsoft SQL Server for the OMNIS Software. Setting up the dedicated Microsoft SQL Server and the database is the responsibility of the internal IT administrator of the user.

Instructions for preparing the external database for use on the OMNIS Server: *Preparing the database*

Instructions on setting up the database on the OMNIS Server: *Setting up a database on the OMNIS Server*

It is not possible to switch from a local database to an external database in the **OMNIS Client/Server system**. The OMNIS Server must be connected to an external database during the initial installation. Likewise, no local database already in use can be transferred from **OMNIS Stand-Alone** to an **OMNIS Client/Server system** or restored there.

In offline mode, the OMNIS Client can access solely the locally available data. Automatic synchronization of the generated and modified data takes place as soon as the OMNIS Client is connected to the OMNIS Server again. The offline mode is only provided for exceptional situations (e.g. if the OMNIS Server is temporarily unavailable for technical reasons).

See also

Backing up the database (chapter 6.1.3, page 1218)

Changing the operation mode (chapter 6.1.8, page 1233)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Database Administration – Actions (chapter 6.1, page 1207)

Operation mode – Definition (chapter 6.1.7, page 1233)

Resetting the local database (OMNIS Stand-Alone and OMNIS Client) (chapter 6.1.5, page 1227)

Restoring the database (chapter 6.1.4, page 1225)

Setting up a database (OMNIS Stand-Alone) (chapter 4.6.1, page 119)

Updating the database (OMNIS Stand-Alone) (chapter 6.1.1, page 1208)

User rights – Directory (chapter 4.5.7.4, page 89)

4.6.1 Setting up a database (OMNIS Stand-Alone)

On initial installation of the OMNIS Software, you can choose between a **local database (Microsoft SQL Server Express)** or a connection to an **external database (dedicated Microsoft SQL Server)**:

- **Local database**: If the local database has been selected, then no further setup steps are necessary. The local database **Microsoft SQL Server Express** is set up on the computer at the time of initial installation of the OMNIS Software.
  After installation from a local database, it is possible to switch to an external database. Observe the following instructions: *Change from a local database to an external database*.

- **Externe Datenbank**: If the external database is selected, then an empty database first has to be set up on a dedicated Microsoft SQL Server for the OMNIS Software. Observe the following instructions: *Setting up a connection to the external database*
  - After setting up the external database, it is no longer possible to switch to a local database.
  - After setting up the external database, the connection settings can be changed. To do this, observe the following instructions: *Changing connection settings*

It is **not** possible to switch from a local database to an external database in the **OMNIS Client/Server system**. The OMNIS Server must be connected to an external database during the initial installation. When using the **OMNIS Client/Server system**, the database must be set up according to the following instructions: *Setting up a database on the OMNIS Server*

Information on the OMNIS Client/Server system: *OMNIS Client/Server system - Definition*

To perform service activities, a total of 3 operation modes of the OMNIS system must be configured. The setup of the database must be carried out for each operation mode separately.

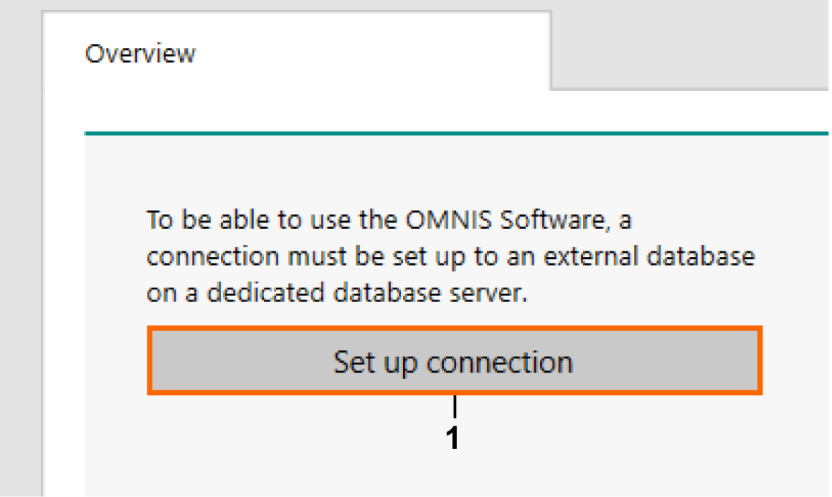
Setting up a connection to the external database on a dedicated Microsoft SQL Server

Prerequisite:

- The Windows user currently logged on has the local administrator rights.
- The options **Stand-alone** and **Dedicated Microsoft SQL Server** were selected on initial installation of the OMNIS Software.
- The **OMNIS Database Administration** program is open.
- The external database is set up for use in the OMNIS Software in accordance with the instructions: *Preparing the database*
- If Windows authentication mode is used, then the user created in *Prepare database (OMNIS Stand-Alone)* must be logged into the Metrohm Miami LabLogic service. Additional information: *(see "Service login", chapter 4.7, page 136)*
- The required operation mode was selected.

1 Starting the setup

- Click on **[Set up connection]** to start the wizard (**1**).



A dialog is opened.

2 Entering data

Application errors may occur if the data entered uses a connection to a database that is already in use. No other user may use the same database at the same time.

Fill in the fields in the dialog (**1**):

- **Database server**: The address must have the following format: **Database server address\instance, port** (e.g. 192.168.1.1\myDatabaseServer, 1433)
  If no default values are used for the instance and the port on the database server, then **instance** and **port** must be entered as specified in the previous example. The required port (default value: 1433) must also be open for access.
- **Database name**

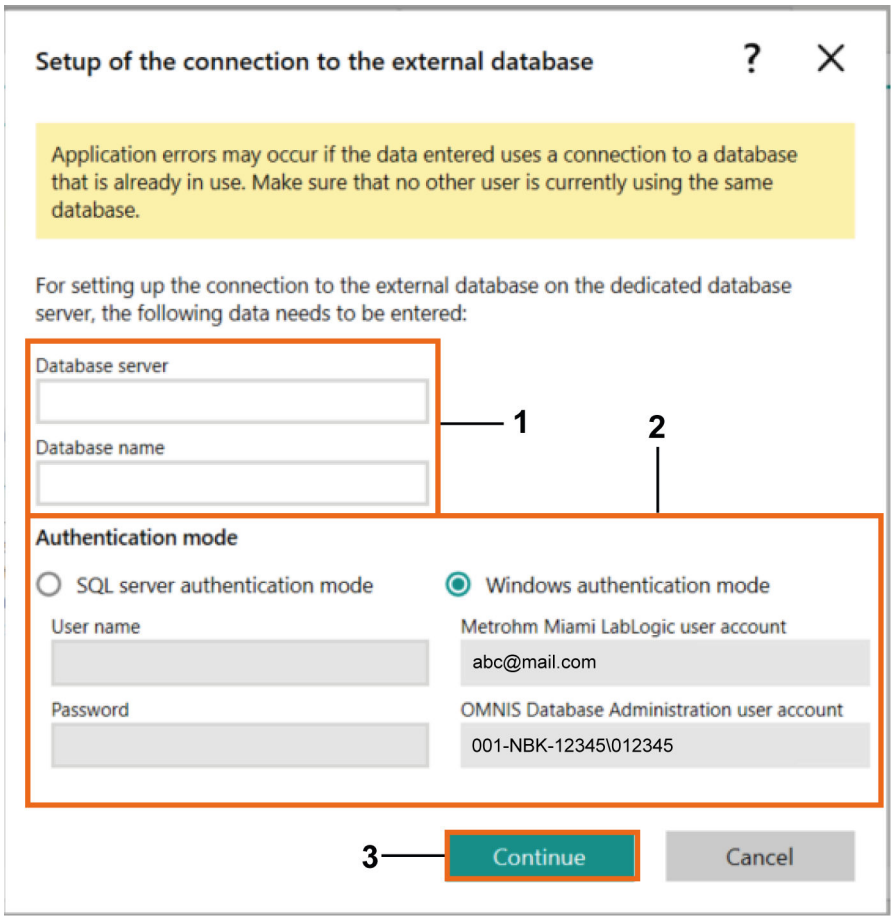
Select the Authentication mode (**2**):

- **SQL server authentication mode**: The connection to the database server is established using the login data defined in Microsoft SQL Server Management Studio.
  - **User name**
  - **Password**

- **Windows authentication mode**: The connection to the database server is established with the Windows user account that is logged into the Metrohm Miami LabLogic service. The server connection is tested with the OMNIS Database Administration user account.
  The login data for Windows authentication mode is applied automatically.
  - **Metrohm Miami LabLogic user account**: The Windows user account that is logged into Metrohm Miami LabLogic service.
  - **OMNIS Database Administration user account**: The Windows user account that is logged into OMNIS Database Administration.

The login data is defined for the database owner when the external database was being prepared. Observe step 16 of the following instructions for this: *Preparing the database (OMNIS Stand-Alone)*. The user name must not contain any spaces.

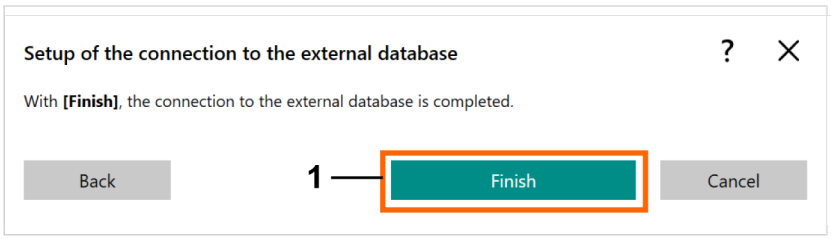
- Click on **[Continue]** (**3**) to continue the setup.



The data entered is validated and the connection to the dedicated database server is continued. A message appears.

3 Completing the setup

- Click on **[Finish]** to confirm the message (**1**) and complete the setup.



The connection to the database server is checked. The connection settings are shown under **OMNIS Database Administration** ▶ **Overview** ▶ **Connection settings** and in the OMNIS Software under **Settings** ▶ **Database settings** ▶ **Connection settings**.

If an external database is used, the **Back up / Restore** tab in the **OMNIS Database Administration** program is not available. Restoring the database and backing up the database must be carried out by an internal IT administrator.

4 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

A message appears if the connection between the OMNIS Software and the database server is interrupted. The OMNIS instruments are stopped automatically. The OMNIS Software needs to be closed and restarted manually to continue working with it.

Switching from a local to an external database

Prerequisite:

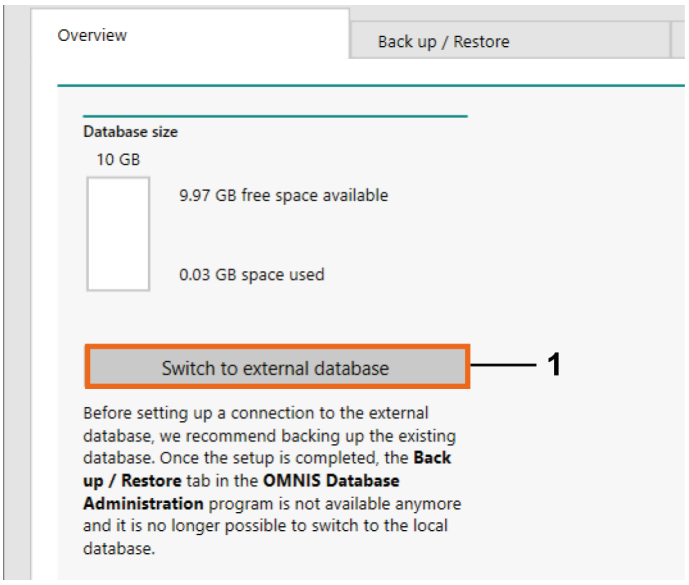
- The Windows user currently logged on has the local administrator rights.
- The options **Stand-alone** and **Dedicated Microsoft SQL Server** were selected on initial installation of the OMNIS Software.
- The **OMNIS Database Administration** program is open.

- The local database on the dedicated database server has been transferred according to the instructions: *Transferring the database*
- If Windows authentication mode is used, then the user created in *Prepare database (OMNIS Stand-Alone)* must be logged into the Metrohm Miami LabLogic service. Additional information: *(see "Service login", chapter 4.7, page 136)*
- The required operation mode was selected.

1 Switching to the external database

Before setting up a connection to the external database, Metrohm recommends backing up the existing database. Once the setup is completed, the **Back up / Restore** tab in the **OMNIS Database Administration** program is not available anymore and it is no longer possible to switch to the local database. Restoring the database and backing up the database must be carried out by an internal IT administrator if an external database is used.

- Click on **[Switch to external database]** under **OMNIS Database Administration** ▶ **Overview** to start the wizard and to switch from the local to the external database (**1**).



2 Entering data

Application errors may occur if the data entered uses a connection to a database that is already in use. Check whether any other user is currently using the same database.

Fill in the fields in the dialog (**1**):

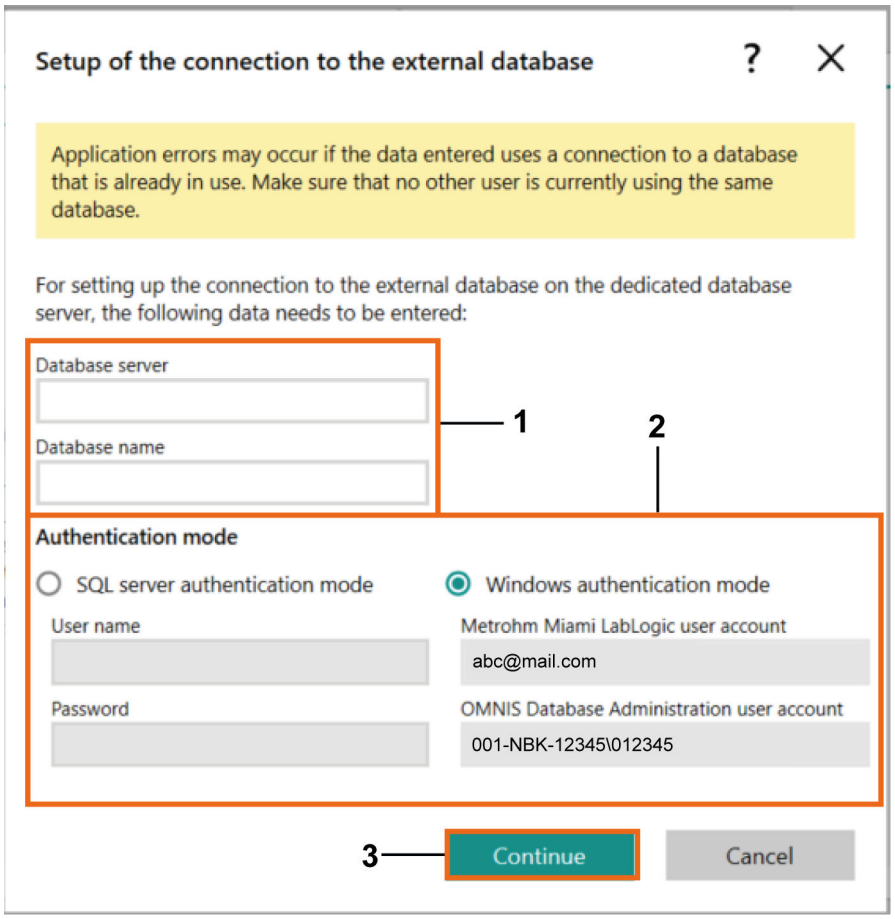
- **Database server**: The address must have the following format: **Database server address\instance, port** (e.g. 192.168.1.1\myDatabaseServer, 1433)
  If no default values are used for the instance and the port on the database server, then **instance** and **port** must be entered as specified in the previous example. The required port (default value: 1433) must also be open for access.
- **Database name**

Select the Authentication mode (**2**):

- **SQL server authentication mode**: The connection to the database server is established using the login data defined in Microsoft SQL Server Management Studio.
  - **User name**
  - **Password**
- **Windows authentication mode**: The connection to the database server is established with the Windows user account that is logged into the Metrohm Miami LabLogic service. The server connection is tested with the OMNIS Database Administration user account.
  The login data for Windows authentication mode is applied automatically.
  - **Metrohm Miami LabLogic user account**: The Windows user account that is logged into Metrohm Miami LabLogic service.
  - **OMNIS Database Administration user account**: The Windows user account that is logged into OMNIS Database Administration.

The login data is defined for the database owner when the external database was being prepared. Observe step 16 of the following instructions for this: *Preparing the database (OMNIS Stand-Alone)*. The user name must not contain any spaces.

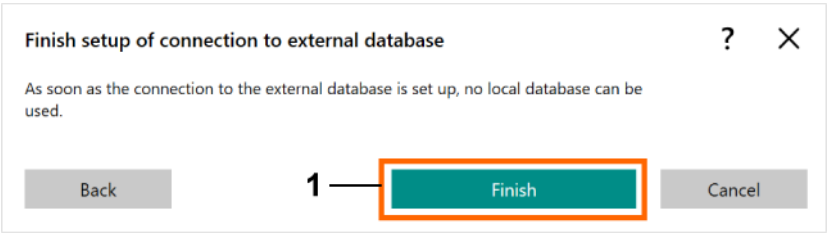
- Click on **[Continue]** (**3**) to continue the setup.



The data entered is validated and the connection to the dedicated database server is continued. A message appears.

3 Completing the setup

- Click on **[Finish]** to confirm the message (**1**). The local database can no longer be used.



The connection to the database server is checked. The connection settings are shown under **OMNIS Database Administration ▶ Overview ▶ Connection settings** and in the OMNIS Software under **Settings ▶ Database settings ▶ Connection settings**.

4 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

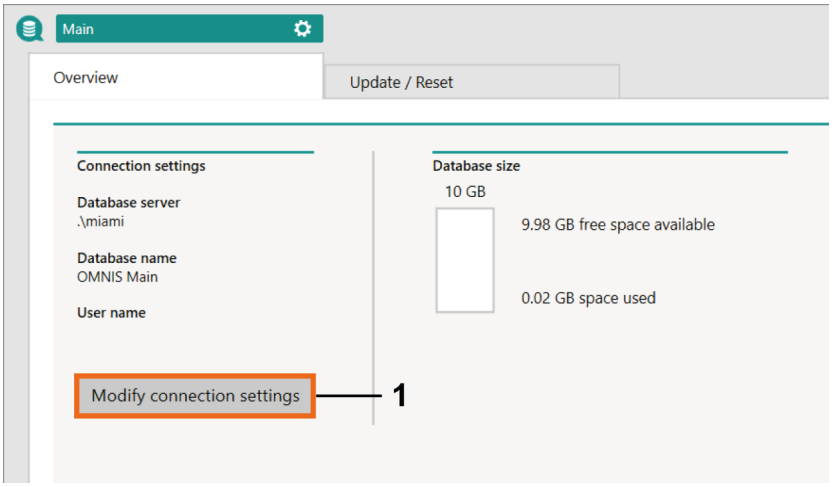
Modifying the connection settings

Prerequisite:

- The options **Stand-alone** and **Dedicated Microsoft SQL Server** were selected on initial installation of the OMNIS Software.
- The external database is installed and in use.
- If Windows authentication mode is used, then the user created in *Prepare database (OMNIS Stand-Alone)* must be logged into the Metrohm Miami LabLogic service. Additional information: *(see "Service login", chapter 4.7, page 136)*
- The required operation mode was selected.

1 Modifying the connection settings

- Click on **[Modify connection settings]** (**1**) under **OMNIS Database Administration ▶ Overview ▶ Connection settings** to change the connection settings for the external database.



The wizard is opened where the data **Database server**, **Database name**, authentication mode and the login data can be changed.

See also

Database – Definition (chapter 4.6, page 117)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Database Administration – Actions (chapter 6.1, page 1207)

Resetting the local database (OMNIS Stand-Alone and OMNIS Client) (chapter 6.1.5, page 1227)

Restoring the database (chapter 6.1.4, page 1225)

Updating the database (OMNIS Stand-Alone) (chapter 6.1.1, page 1208)

User rights – Directory (chapter 4.5.7.4, page 89)

4.6.2 Setting up a database (OMNIS Client/Server system)

To perform service activities, a total of 3 operation modes of the OMNIS system must be set up. Proceed as follows:

1. Perform steps 1-4 of the instructions for the **Main** operation mode.
2. Repeat steps 1-4 for the **OQ-FS** operation mode.
3. Repeat steps 1-4 for the **C1-PV** operation mode.

The individual steps of the instructions must **not** be carried out simultaneously for several operation modes.

Additional information on the operation modes: *Definition operation mode*

If the **OMNIS Client/Server system** is used, each OMNIS Client works with the local database and synchronizes automatically with the OMNIS Server. The OMNIS Server works with an external database on which generated data is centrally stored. In offline mode, the OMNIS Client can access solely the locally available data. All created and changed data is saved to the local database. Automatic synchronization takes place as soon as the OMNIS Client is connected to the OMNIS Server again. The option to work in offline mode is provided only in exceptional situations (e.g. if the OMNIS Server is temporarily unavailable for technical reasons).

Information on the **OMNIS Client/Server system**: *OMNIS Client/Server system - Definition*

Setting up the database connection on the OMNIS Server

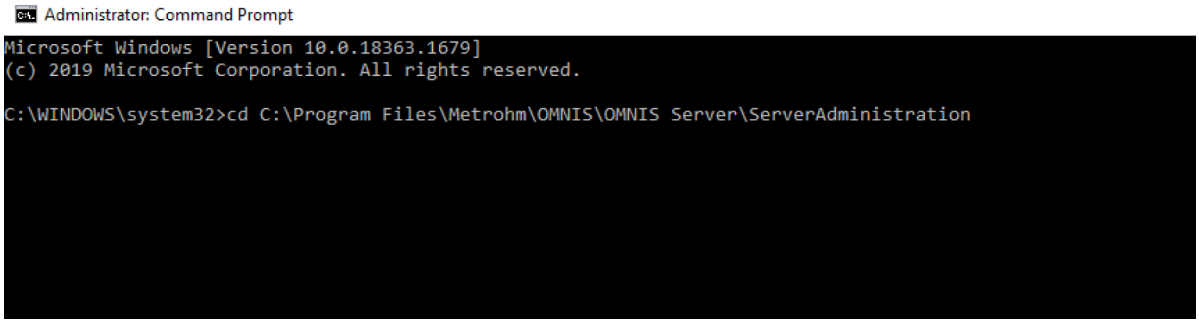
Prerequisite:

- The Windows user currently logged on has the local administrator rights.
- The options **OMNIS Client/Server**, **Server including 1 client** and **Dedicated Microsoft SQL Server** were selected on initial installation of the OMNIS Software: *Installing the OMNIS Software*
- The external database is set up for the use in the OMNIS Software according to the instructions:
  Preparing the database (OMNIS Client/Server system)

It is not possible to switch from a local database to an external database in the **OMNIS Client/Server system**. The OMNIS Server must be connected to an external database during the initial installation.

1 Switching to the OMNIS Server in a command prompt

- Open the Windows start menu.
- Search for the Windows command prompt. Open the context menu by right-clicking and select **Run as administrator**.
- Enter the text **cd** (change directory) followed by a space and then enter the installation pathway of the OMNIS Server (**C:\Program Files\Metrohm\OMNIS\OMNIS Server\ServerAdministration** by default).
- Confirm the entry with **[Enter]**.



2 Configuring the connection via command prompt

All the necessary access data can be obtained from the internal IT administrator.

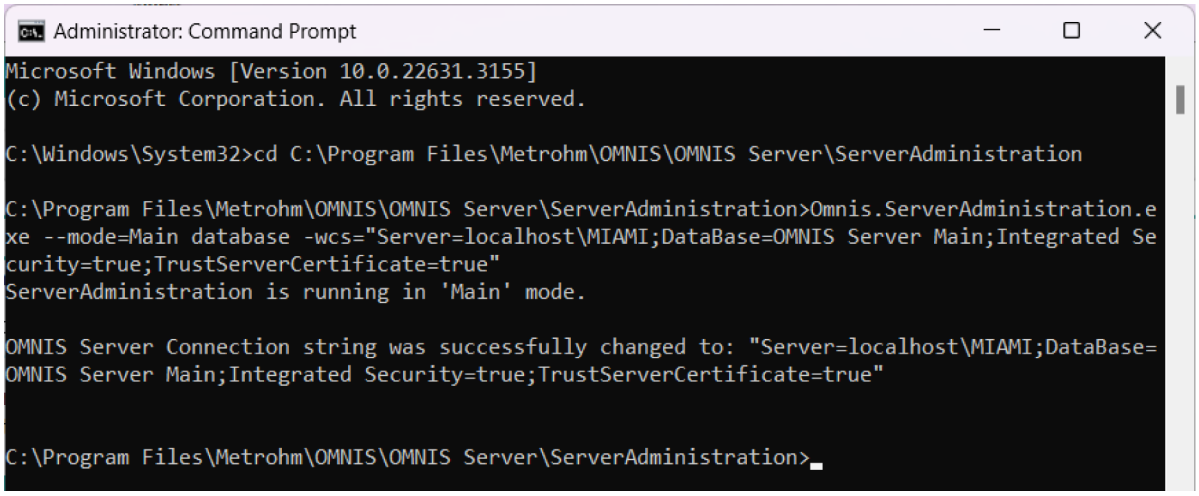
Encryption is activated by default for the connection between the OMNIS server and the database server. The certificate to be used must have been issued by a trusted certificate authority. If required (e.g. for use in a test environment), you can also work with self-signed certificates by adding the parameter **";TrustServerCertificate=true"** for the definition of the database connection parameters. For safety reasons, Metrohm recommends not using self-signed certificates in production environments, as they do not offer high safety standards.

If the Windows authentication mode was selected in the following instructions *Preparing the database (OMNIS Client/Server system)* **(recommended)**:

- Prepare the following information:
  - Name of the computer in the network on which the Microsoft SQL Server is running (e.g. 001-CMP-00000).
  - Instance of the Microsoft SQL Server (e.g. METROHM-SERVER). When using the standard server instance, no instance needs to be specified in place of **MSSQLSERVER** or **MSSQL** (e.g. Server=**Name of the computer**\;DataBase=**Name of the database**;)
  - Name of the database (Main, OQ-FS or C1-PV) on the Microsoft SQL Server (e.g. OMNISServer).
  - Specification of the user authentication. If Integrated Security is set to true, then Windows authentication is used.
  - Specification of the certificate type (self-signed or acquired from a trusted certificate authority).
- Enter the following text line in the command prompt, replacing the individual text parts with your own specific information:
  Omnis.ServerAdministration.exe --mode=**Name of the operation mode** database -wcs="Server=**Name of the computer\Server instance**;DataBase=**Name of the database**;IntegratedSecurity=**true**"
  Example for the entry in the Main operation mode:
  - Omnis.ServerAdministration.exe --mode=Main database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerMain;IntegratedSecurity=true"

  Example for the entry in the OQ-FS operation mode in the second run of the instructions:
  - Omnis.ServerAdministration.exe --mode=OQ-FS database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerOQ-FS;IntegratedSecurity=true"

  Example for the entry in the C1-PV operation mode in the third run of the instructions:
  - Omnis.ServerAdministration.exe --mode=C1-PV database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerC1-PV;IntegratedSecurity=true"
- Confirm the entry with **[Enter]**.



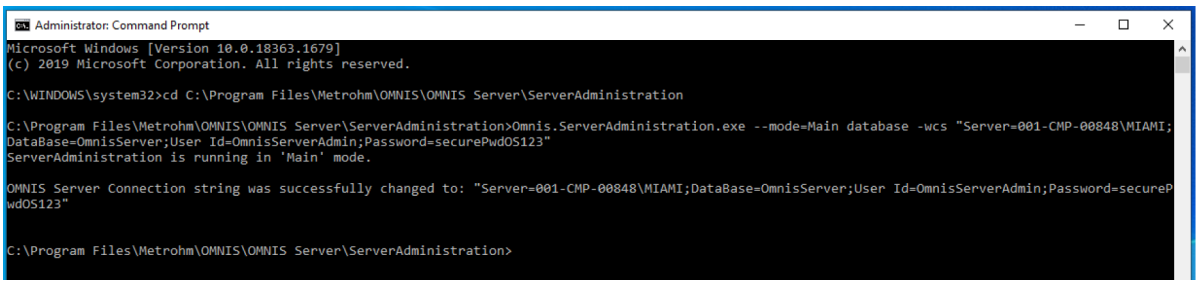
If the SQL server authentication mode was selected in the following instructions *Preparing the database (OMNIS Client/Server system)*:

- Prepare the following information:
  - Name of the computer in the network on which the Microsoft SQL Server is running (e.g. 001-CMP-00000).
  - Instance of the Microsoft SQL Server (e.g. METROHM-SERVER).
  - Name of the database (Main, OQ-FS or C1-PV) on the Microsoft SQL Server (e.g. OMNISServer).
  - Name of the user for the access to the database (e.g. OMNISServerAdmin).
  - Password of the user for access to the database (e.g. OMNISServerAdminPassword).
  - Specification of the certificate type (self-signed or acquired from a trusted certificate authority).

- Enter the following text line in the command prompt, replacing the individual text parts with your own specific information:
  Omnis.ServerAdministration.exe --mode=**Name of the operation mode** database -wcs="Server=**Name of the computer\Server instance**;DataBase=**Name of the database**;User Id=**Name of the user**;Password=**Password of the user**"
  Example for the entry in the Main operation mode:
  – Omnis.ServerAdministration.exe --mode=Main database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerMain;User ID=OMNISServerAdmin;Password=OMNISServerAdminPassword"

  Example for the entry in the OQ-FS operation mode in the second run of the instructions:
  – Omnis.ServerAdministration.exe --mode=OQ-FS database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerOQ-FS;User ID=OMNISServerAdmin;Password=OMNISServerAdminPassword"

  Example for the entry in the C1-PV operation mode in the third run of the instructions:
  – Omnis.ServerAdministration.exe --mode=C1-PV database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerC1-PV;User ID=OMNISServerAdmin;Password=OMNISServerAdminPassword"
- Confirm the entry with **[Enter]**.



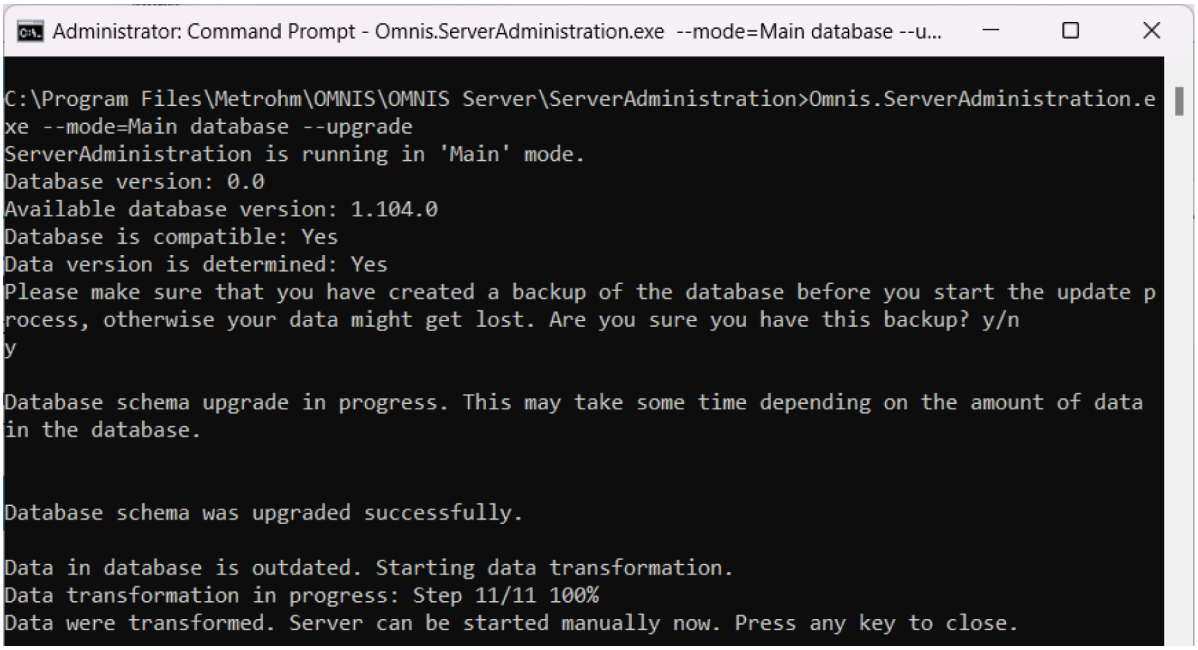
The command prompt confirms that the connection was successfully changed.

3 Creating a database schema

- Enter the following text in the command prompt:
  Example for the entry in the Main operation mode:
  – Omnis.ServerAdministration.exe --mode=Main database --upgrade

  Example for the entry in the OQ-FS operation mode in the second run of the instructions:
  – Omnis.ServerAdministration.exe --mode=OQ-FS database --upgrade

  Example for the entry in the C1-PV operation mode in the third run of the instructions:
  – Omnis.ServerAdministration.exe --mode=C1-PV database --upgrade
- Confirm the entry with **[Enter]**.



The command prompt confirms that the database schema was successfully created.

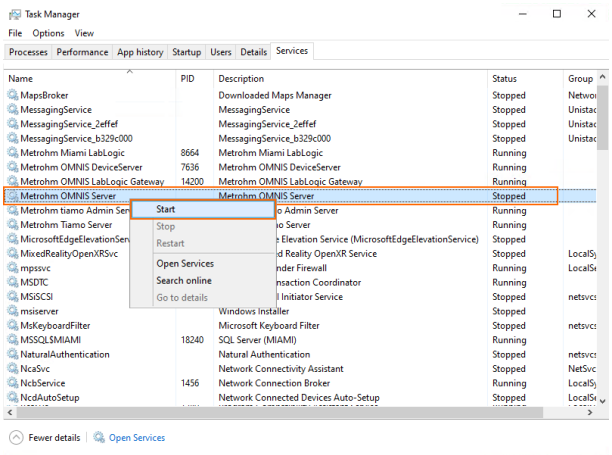
4 Starting the service for the OMNIS Server

- Right-click on the Windows task bar and select **[Task Manager]** in the selection list.

- Right-click on the applicable service on the **Services** tab:
  Main operation mode:
  – Service **Metrohm OMNIS Server**

  OQ-FS operation mode in the second run of the instructions:
  – Service **Metrohm OMNIS Server_OQ-FS**

  C1-PV operation mode in the third run of the instructions:
  – Service **Metrohm OMNIS Server_C1-PV**
- Select **[Start]** in the selection list.



The service is started.

The following reasons may apply if the **Metrohm OMNIS Server** (**Metrohm OMNIS Server_OQ-FS** or **Metrohm OMNIS Server_C1-PV)** service cannot be started:

- The database schema is not up-to-date or not compatible with the OMNIS Server.
- The connection to the database could not be established.

If this is the case, then check the data entered in the command prompt according to step 2 (Configuring the connection via command prompt). To check the database connection, the following text can be entered in the command prompt:
Omnis.ServerAdministration.exe --mode=**Name of the operation mode** database --info
Enter the data for the connection again, if applicable. Contact your internal IT administrator if this error continues to occur.

5 Creating a local database (OQ-FS and C1-PV)

During initial installation, only the "Main" local database is installed automatically. The local databases for C1-PV and OQ-FS must be created manually on a one-time basis. The local databases are necessary for the offline mode and must be present.

- Open the **OMNIS Database Administration** program.
- Change the operation mode (**OQ-FS** or **C1-PV**).
- In the message that the database must be reset, create a new database by clicking on **[Reset]**.

6 Repeating the instructions

- Repeat all the steps in the second and third run for the corresponding operation mode.

7 Activating the software license

- Start the OMNIS Software.
- Activate the software license by following these instructions: *(see "Activating the software license", chapter 4.2.1, page 29)*

See also

Changing the operation mode (chapter 6.1.8, page 1233)

Database – Definition (chapter 4.6, page 117)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Database Administration – Actions (chapter 6.1, page 1207)

Operation mode – Definition (chapter 6.1.7, page 1233)

Resetting the local database (OMNIS Stand-Alone and OMNIS Client) (chapter 6.1.5, page 1227)

Restoring the database (chapter 6.1.4, page 1225)

Updating the database (OMNIS Stand-Alone) (chapter 6.1.1, page 1208)

User rights – Directory (chapter 4.5.7.4, page 89)

4.7 Service login

Logging in via Services

Prerequisite:

- The OMNIS Software is installed.
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The Windows user currently logged on has the local administrator rights.
- The group directives are edited according to the instructions: *Start services*

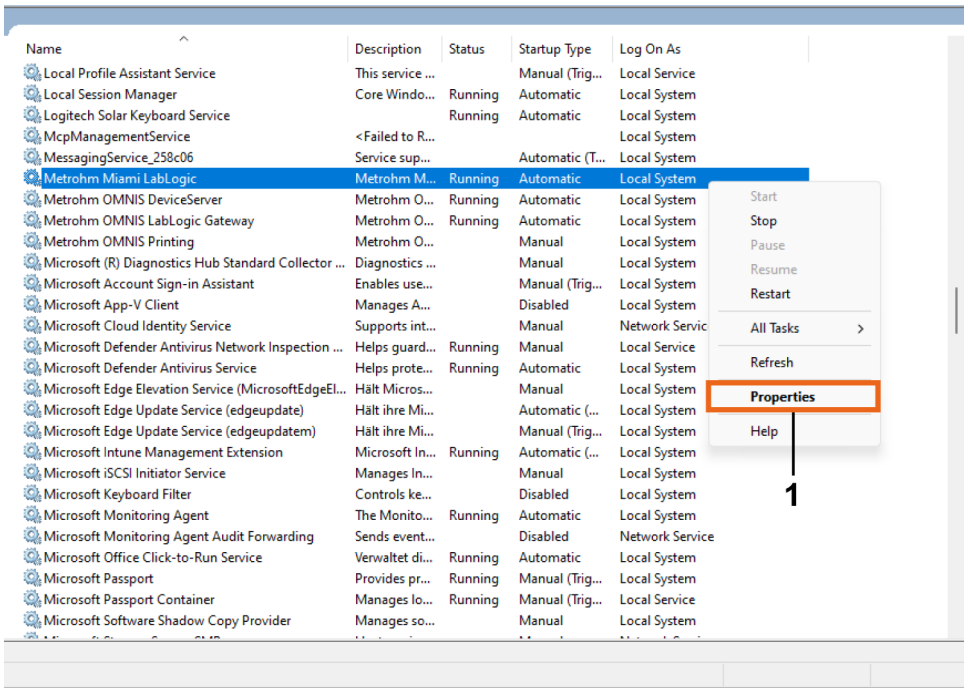
1 Opening the services

- Open the Windows start menu.
- Search for and select **Services**.

A new window is opened.

2 Opening the properties

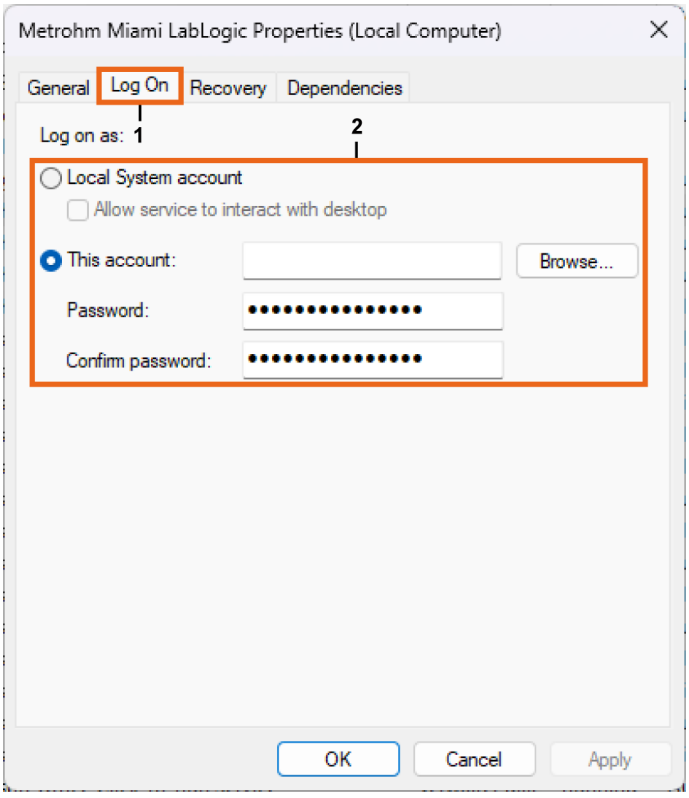
- Right-click on the corresponding service and select **[Properties]** in the selection list.



A new window is opened.

3 Logging into the service

- Under **Login (1)**, select the option **This account (2)**.
- Enter the account or click on **[Search...]** to search for it and assign a password. Confirm the password once more.
- Click on **[OK]** to confirm the entry.



A new window is opened.

4 Restarting the service

- Right-click on the corresponding service and select **[Restart]** in the selection list.

4.8 Assigning IP addresses

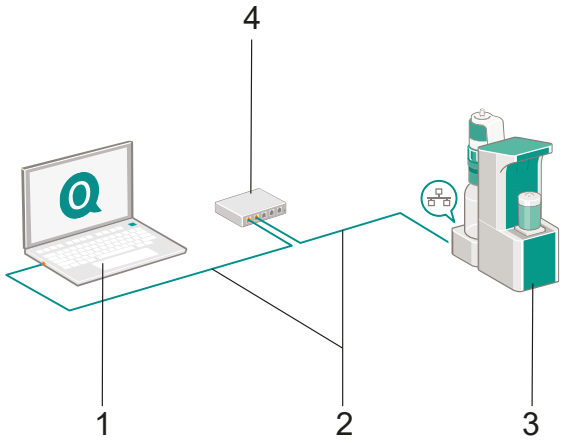
Using the **OMNIS device TCP/IP Service Port** of an OMNIS instrument makes it possible to change the address assignment from a dynamic IP address (automatic IP-address assignment via DHCP) to a static IP address.

Furthermore, the user can use the **OMNIS device TCP/IP Service Port** to define an individual host name for an OMNIS instrument.

- *Typical components of a network with LAN cable connection*
- *Identifying a previously assigned IP address with connected DHCP server*
- *Resetting a previously assigned static IP address without DHCP server*
- *Changing from static IP address to dynamic IP address*
- *Assigning a static IP address*
- *Assigning a dynamic IP address*
- *Defining an individual host name*

Typical components of a network with LAN cable connection

The IP address of an OMNIS instrument is set to **dynamic** DHCP in the factory settings.



1 **Computer** A computer with OMNIS Software installed.	**2** **LAN cable connections** A LAN cable connection with a category 5 cable or higher.
3 **OMNIS instrument** The OMNIS instrument (e.g. OMNIS Titrator).	**4** **Ethernet Router** An Ethernet Router for providing IP addresses via the DHCP communications protocol.

Identifying a previously assigned IP address with connected DHCP server

Prerequisite:

- The latest version of a browser is installed.
- OMNIS Software version 2.7 or higher is installed and the OMNIS instrument has the corresponding firmware version.

1 Switching on and connecting the Ethernet Router

- Switch on the Ethernet Router and wait until it is ready for operation.
- Connect the OMNIS instrument to the Ethernet Router.

2 Starting the OMNIS Software

- Start the OMNIS Software.

3 Switching on the OMNIS instrument

- Switch on the OMNIS instrument and wait until an acoustic signal (bleep) is heard.

4 Opening instrument management

- Click on to open the **Inventory** window in **Equipment ▶ Instruments**.

5 Searching for an instrument

- Click on if new instruments have been connected.
- Enter the desired search criterion (name and type) in the search field.

The instrument list will display only the instruments which contain the search term used.

6 Identifying the IP address

- Place the cursor on the OMNIS instrument you are looking for in the Inventory.
- Note the **IP address and port of the instrument** that is displayed in the tooltip (e.g. 192.168.1.101:9116).

Resetting a previously assigned static IP address without DHCP server

If a static IP address has been assigned to the OMNIS instrument, but this is no longer known, then the IP address must be reset to the factory settings. To do this, the OMNIS instrument must be switched off and back on again several times.

Resetting the IP address to factory settings only works if the IP settings of an OMNIS instrument have been set to **static**.

1 Switching off the OMNIS instrument

- Switch off the OMNIS instrument.

2 Restarting the OMNIS instrument

- Wait 5 seconds and then switch the OMNIS instrument back on again.

Wait until an acoustic signal (bleep) is heard from the OMNIS instrument.

3 Repeating the steps

- Repeat steps 1 and 2 five times within 8 minutes.
- Repeat steps 1 and 2 again. The changes take effect only after the 6th time.

The IP address and network mask are reset to the factory settings of the OMNIS instrument: IP address 192.168.10.1, network mask: 255.255.255.0.

After the reset, the OMNIS instrument still has a static IP address without DHCP server. Additional information on changing to static IP address with DHCP server: *Changing from static IP address to dynamic IP address*

Changing from static IP address to dynamic IP address

Prerequisite:

- The latest version of a browser is installed.
- OMNIS Software version 2.7 or higher is installed and the OMNIS instrument has the corresponding firmware version.

- The OMNIS instrument must be connected by a LAN cable connection.

1 Restarting the OMNIS instrument

- Wait for the OMNIS instrument to restart, until an acoustic signal (beep sound) is heard from the OMNIS instrument.

2 Unplugging the LAN cable

- Unplug the LAN cable from the OMNIS instrument.
- Wait 5 seconds.

3 Plugging in the LAN cable

- Plug the LAN cable into the OMNIS instrument.
- Wait 3 seconds.

4 Repeating the steps

- Repeat steps 2 and 3 five times within 3 minutes.
- Repeat steps 1 and 2 again. The changes take effect only after the 6th time.

The OMNIS instrument was changed to the dynamic IP address.

Assigning a static IP address

Prerequisite:

- The latest version of a browser is installed.
- The OMNIS instrument is connected to an Ethernet Router with an active DHCP server.
- OMNIS Software version 2.7 or higher is installed and the OMNIS instrument has the corresponding firmware version.

1 Opening the browser

- Open a current browser.
- Enter the link *http://{IP address}:8080* in the address line and, for the **IP address**, enter the IP address noted in the last section (*Identifying a previously assigned IP address with connected DHCP server*). Example: *http://10.0.34.63:8080*
- Confirm the address by clicking on **[Enter]**.

A new window is opened.

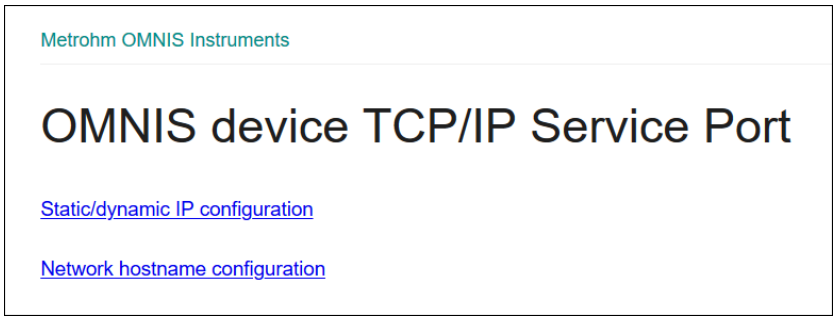
2 Entering the user name and the password

- In the window, enter **MetServTech** as **User name** and **MCh91*Serv** as **Password**.

- Click on **[OK]** to confirm the entry.

3 Selecting an option

- Select the option **Static/dynamic IP configuration** for setting an IP address.

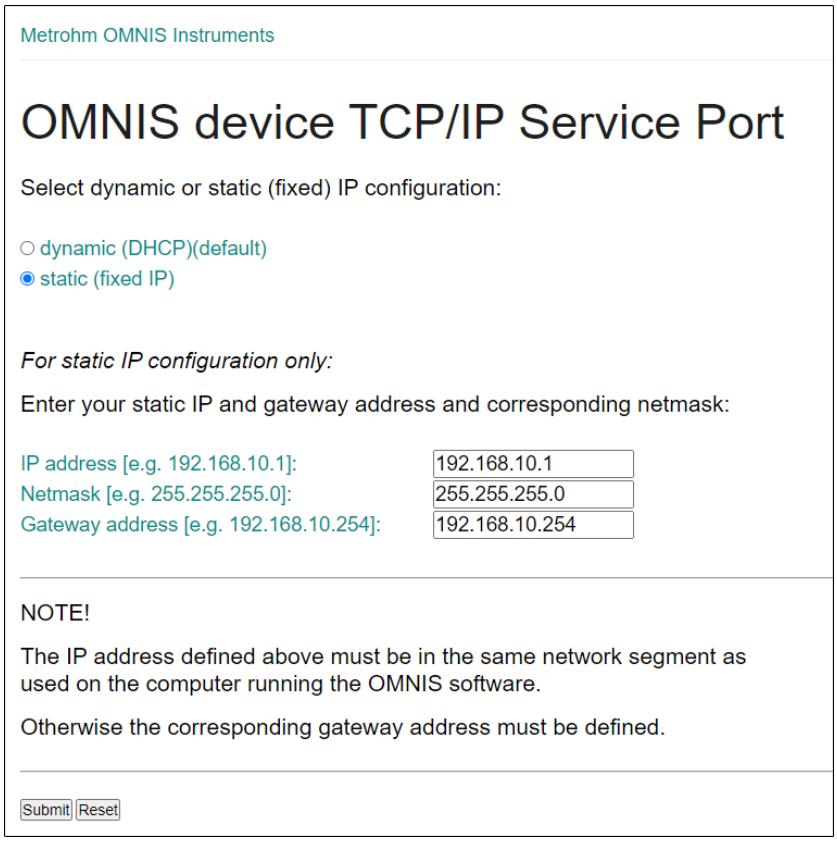


A new window is opened.

4 Entering an IP address

- Select the option **static (fixed IP)** for setting a fixed IP address.
- Under **IP address**, enter the desired IP address.
- Under **Netmask**, enter a matching netmask.
- Under **Gateway address**, enter the IP address of the connection gateway used if the device is located in a subnet different from the one containing the computer being used.
- Click on **[Submit]** to confirm the entries.

The IP address 0.0.0.0 is invalid.
Clicking on **[Submit]** repeatedly can cause an error. If an error message is displayed, then the respective OMNIS instrument needs to be restarted.



The new IP settings do not take effect until after restarting the OMNIS instrument (switch off and then switch back on again).

To find the OMNIS instrument in the network automatically, the IP address defined above must be on the same network as the computer on which the OMNIS Software is being run. If the OMNIS instrument and the computer with the OMNIS Software are in different subnets, then the connection can be configured manually.

Assigning a dynamic IP address

Prerequisite:

- The latest version of a browser is installed.
- The OMNIS instrument is connected to an Ethernet Router with an active DHCP server.

- OMNIS Software version 2.7 or higher is installed and the OMNIS instrument has the corresponding firmware version.

1 Opening the browser

- Open a current browser.
- Enter the link *http://{IP address}:8080* in the address line and, for the **IP address**, enter the IP address noted in the last section (*Identifying a previously assigned IP address with connected DHCP server*). Example: *http://10.0.34.63:8080*
- Confirm the address by clicking on **[Enter]**.

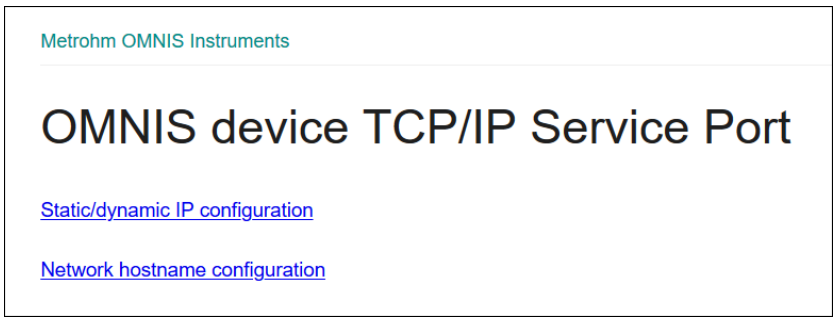
A new window is opened.

2 Entering the user name and the password

- In the window, enter **MetServTech** as **User name** and **MCh91*Serv** as **Password**.
- Click on **[OK]** to confirm the entry.

3 Selecting an option

- Select the option **Static/dynamic IP configuration** for setting an IP address.

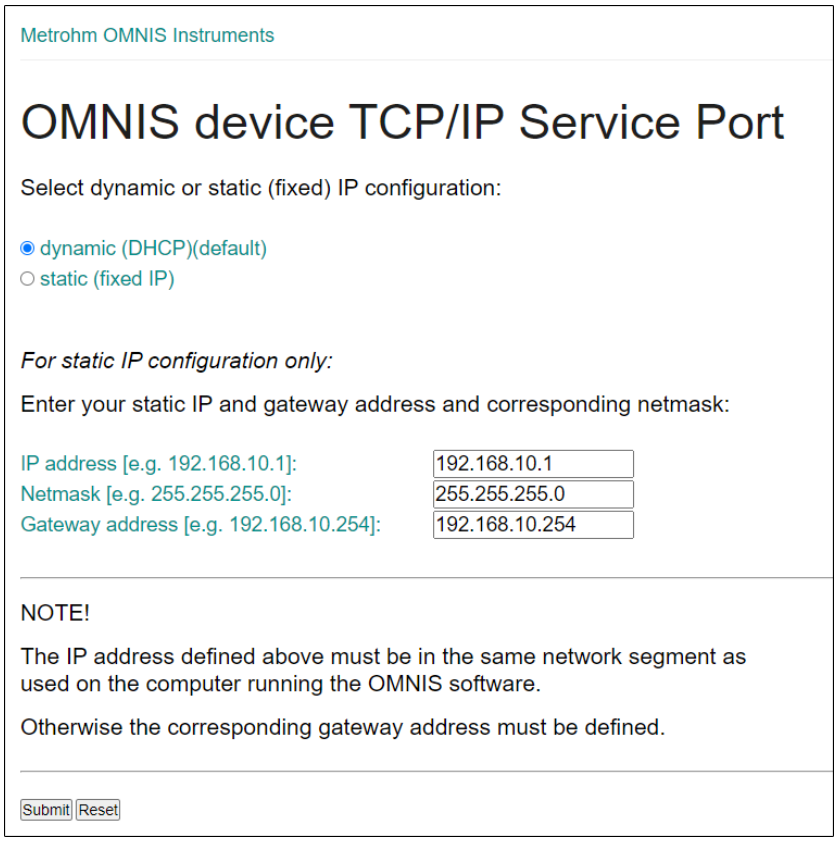


A new window is opened.

4 Entering an IP address

- Select the option **dynamic (DHCP)(default)** for setting a dynamic IP address. The input fields must not be filled out. The DHCP server automatically adopts the correct values.
- Click on **[Submit]** to confirm the entries.

Clicking on **[Submit]** repeatedly can cause an error. If an error message is displayed, then the respective OMNIS instrument needs to be restarted.



The new IP settings do not take effect until after restarting the OMNIS instrument (switch off and then switch back on again).

To find the OMNIS instrument in the network automatically, the IP address defined above must be on the same network as the computer on which the OMNIS Software is being run. If the OMNIS instrument and the computer with the OMNIS Software are in different subnets, then the connection can be configured manually.

Defining an individual host name

Prerequisite:

- The latest version of a browser is installed.
- OMNIS Software version 2.7 or higher is installed and the OMNIS instrument has the corresponding firmware version.

1 Opening the browser

- Open a current browser.

- Enter the link *http://{IP address}:8080* into the address line and at the same time the IP address noted in the preceding **Identify IP address** section as the {IP address}. Example: *http://10.0.34.63:8080*
- Confirm the address by clicking on **[Enter]**.

A new window is opened.

2 Entering the user name and the password

- In the window, enter **MetServTech** as **User name** and **MCh91*Serv** as **Password**.
- Click on **[OK]** to confirm the entry.

3 Selecting an option

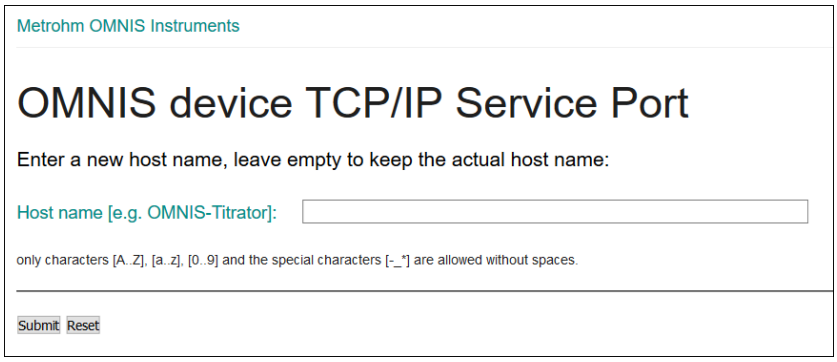
- Select the option **Network hostname configuration** for configuring the instrument name in the network.

A new window is opened.

4 Entering a host name

- Enter the host name of the OMNIS instrument in the **Host name** input field.
- Click on **[Submit]** to confirm the entries.

The host name must contain at least 3 characters.
Clicking on **[Submit]** repeatedly can cause an error. If an error message is displayed, then the respective OMNIS instrument needs to be restarted.



The new host name does not take effect until after restarting the OMNIS instrument (switch off and then switch back on again).

The host name of the OMNIS instrument is reset once again after a firmware update on an OMNIS instrument.

See also

Reserving and releasing instruments (chapter 5.12.2.4, page 861)

4.9 Data exchange with third-party software – Definition

For the data exchange between OMNIS Software and third-party software, OMNIS Software provides a **web API**. Using this interface, third-parties get access to the OMNIS system and can integrate the OMNIS Software into their system.

After configuring this interface and fulfilling the necessary prerequisites for secure data exchange, third-party software (laboratory information systems such as STARLIMS, 1LIMS, etc.) can use the OMNIS Software to interact with sample data and subsample data in the OMNIS system.

Information on configuring the web API: *3rd Party Data Integration API - Technical White Paper*

Prerequisites for secure communication between the OMNIS Software and third-party software:

- **Installation:** API access must be set up during the initial installation using the installation wizard. This defines the ports and the certificate for secure communication. Subsequent API access for existing OMNIS systems is done via the **LaboratoryLogicGateway.exe** program command prompt **(see 3rd Party Data Integration API - Technical White Paper**).

- **Software licenses:** A separate software license is required in the **OMNIS Stand-Alone** or **OMNIS Client/Server system** to access the web API.
- **Authentication and authorization:** The web API supports not only **OAuth 2.0** but also **Basic Authentication** for authentication and authorization. For additional information regarding authentication and authorization, in the **3rd Party Data Integration API – Technical White Paper**.
  - Metrohm recommends the 2-step security process with the aid of the **OAuth 2.0 protocol**. Token-based authentication verifies the identity of the accessing application. Registered applications must present a **Client ID** and a **Client Secret** (secret client key) and receive a unique access token after successful verification. Authentication must be followed by authorization by **User name** and **Password**.
  - Only the user name and the password are required for user authentication with **Basic Authentication**.
- **Technical User and user rights:** Metrohm recommends creating a user for technical purposes only, to enable secure communication between the OMNIS Software and the third-party software. For this so-called Technical User, Metrohm recommends creating a self-defined user group (e.g. Technical Users) and user role (e.g. Technical User). This user role must be assigned all rights that are necessary for API access. Additional information on user rights for API access: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- **Technical User and data permissions:** Data permissions are also applied to the Technical User. With activated data permissions, the data returned by the Web API is filtered according to the data permissions settings of the Technical User. If data is created via the Web API in the OMNIS Software, then data permissions are automatically assigned to this data according to the data permission settings of the Technical User.
- **User management:** The use of the web API requires an enabled user management.

The following rules apply to data exchange with third-party software:

- If the third-party software and an OMNIS user edit the same data at the same time, the changes of the user whose changes were saved first are applied. The other user is informed that his last changes may have to be repeated.

- If a user makes manual changes to a subsample that is being used at the same time in a determination by third-party software, then those changes will be applied from the determination. The results of a determination overwrite the manual changes and the other user is informed that his or her last changes may need to be repeated.
- Metrohm recommends making the following settings for the Technical User in the **Properties** window under **User management** ► **User list**:
  - Enable the **Password never expires** check box.
  - Disable the **Request change of password** check box.

Metrohm recommends using analogous password policies for the Technical User when using **User management with Active Directory integration**.

- To prevent improper access to data, Metrohm recommends never disabling the **Password required** check box under **User management** ► **User management settings**.
- All changes made in the OMNIS Software by the third-party software are recorded and listed in the Audit Trail.

See also

Activating the software license (chapter 4.2.1, page 29)

Audit Trail – Directory (chapter 5.14.5, page 1177)

Data permissions – Definition (chapter 4.5.9, page 105)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

Sending data to third-party software (chapter 5.10.7.8, page 291)

Settings – Actions (chapter 5.15, page 1197)

User groups – Directory (chapter 4.5.6.3, page 84)

User management settings – Subsection (chapter 4.5.4, page 66)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Directory (chapter 4.5.7.3, page 88)

5 Operation and control

5.1 OMNIS Software – System overview

The main focus of the OMNIS Software is directed at the determination of a sample. The preconditions displayed in the overview must be fulfilled in order for a determination to be carried out successfully. Each staircase step of the overview pyramid forms the basis for the staircase step that follows it. This means that the installed hardware (at the very bottom) is the basic precondition for all subsequent areas. The determination of the sample (at the very top) ultimately comprises the entire process.

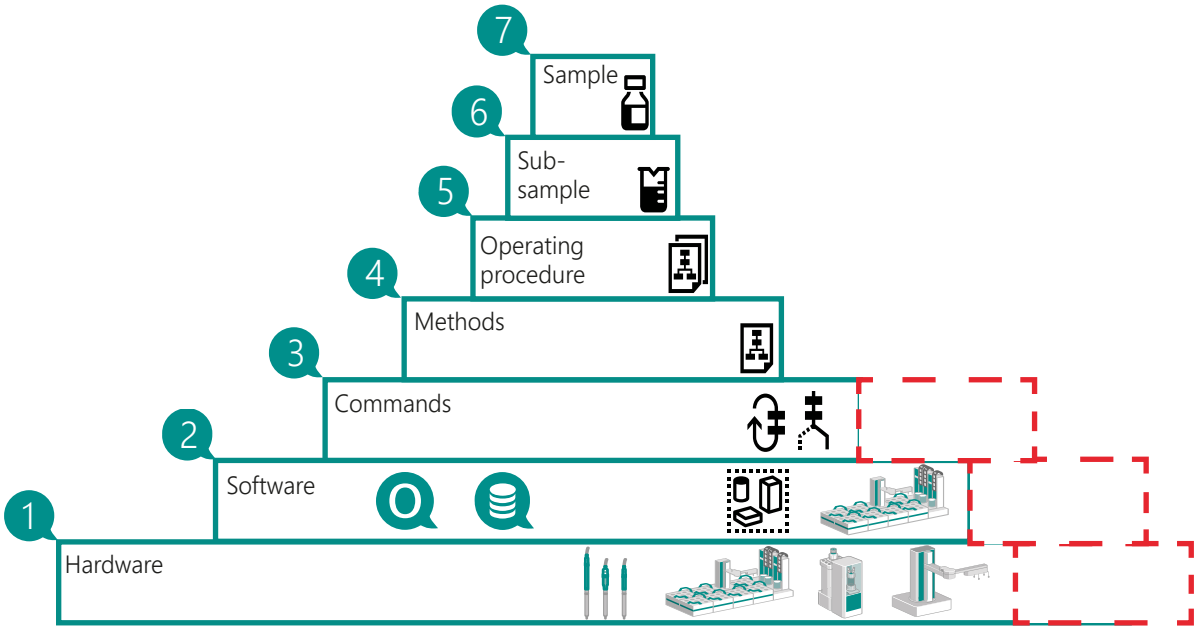


Figure 5 Overview of the OMNIS system from the hardware to the sample.

1 Hardware
Hardware that has been installed and put into operation. Additional instrument functions can be activated in order to enlarge the scope of functions.

2 Software
Software that has been installed and started up. The scope of functions is dependent on the hardware that has been put into operation and the activated licenses.

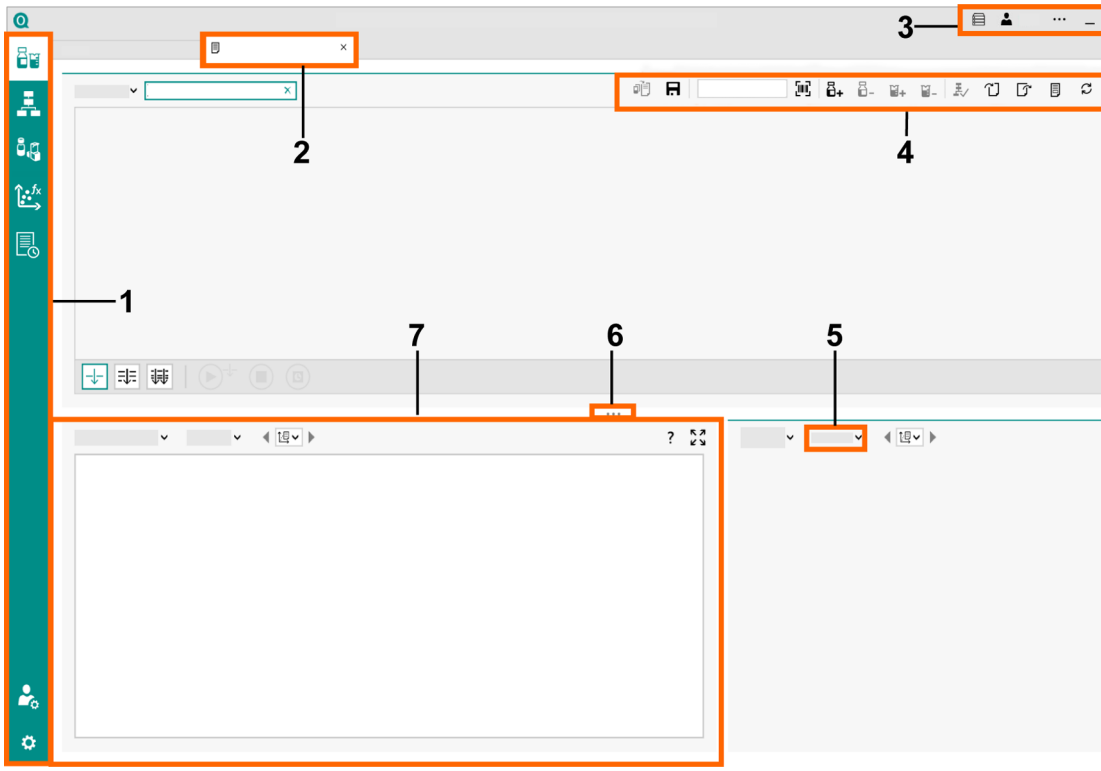
The hardware for the locally running OMNIS Software is reserved in the **Instruments** subsection. The functional units of the reserved instruments are combined into logical work systems that are necessary for the sample determination.

3	**Commands** Commands execute clearly defined tasks. Some commands need to have functional units of a work system assigned to them in order for the commands to be able to carry out their task. The command variables are used to transfer information between the commands.
4	**Methods** Methods are the logical containers for commands. A task area is processed through the combination of several commands within a single method. A minimum of one work system must be assigned to a method in order for that method to be able to accomplish its task.
5	**Operating procedure** The determination run of a subsample is defined and performed with an operating procedure. Operating procedures contain methods and are accessed themselves by subsamples. Multiple methods can be combined either in parallel or in series in an operating procedure.
6	**Subsamples** Subsamples are part of a sample. A different determination can be carried out for each subsample. An operating procedure must be assigned to each subsample for this reason.
7	**Sample** A sample must contain a minimum of one subsample. Samples are presented in a sample list. Templates for the creation of samples and subsamples can be defined through a sample profile.

5.2 User interface OMNIS Software – Overview

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Overview of the user interface



1	**Work areas**	**2**	**Tab**
3	**Title bar (icons for the entire OMNIS Software)**	**4**	**Toolbar (icons for the respective area)**
5	**Subsection**	**6**	**Divider**
7	**Area**		

Work area

The following work areas are displayed on the navigation bar (**1**):

Samples

Processes

Equipment

Models

Audit Trail

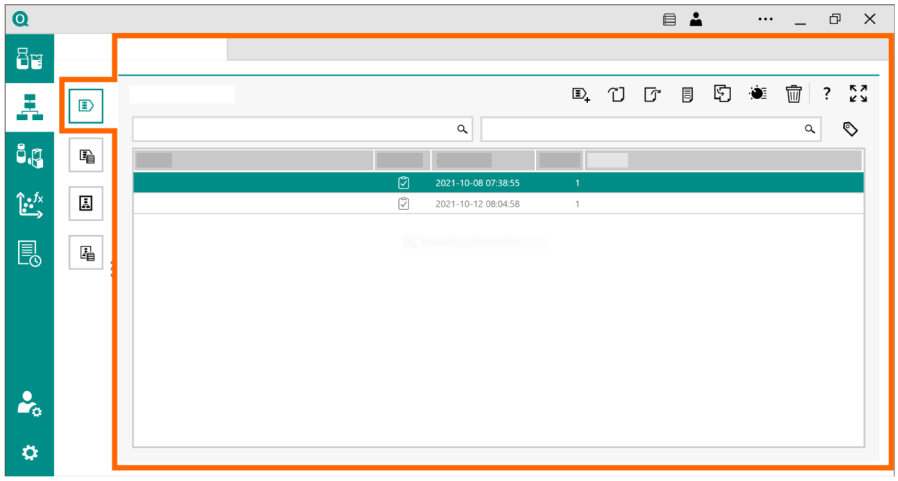
User management

Settings

Subsection

A subsection (**5**) is a subelement of a work area, area or window. You can switch from one subsection to another. It is not possible to open more than one subsection at the same time.

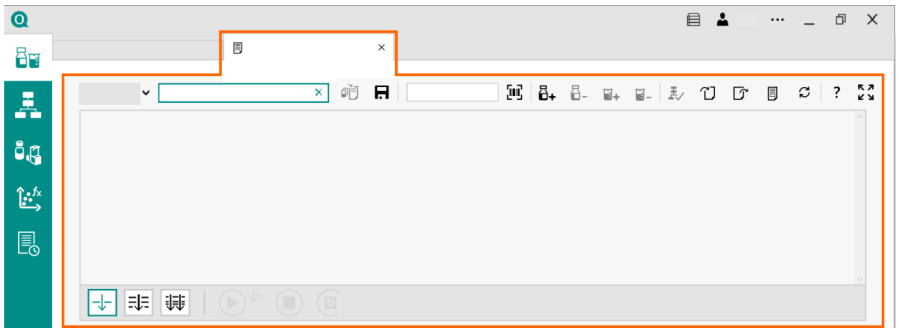
Example: The **Operating procedures** subsection in the **Processes** work area



Tab

A tab (**2**) is opened as soon as a new object (e.g. operating procedure, sample list, etc.) is created. The user can switch between multiple opened tabs. The sequence of the active tabs can be changed per drag and drop. Tabs can also be closed again individually.

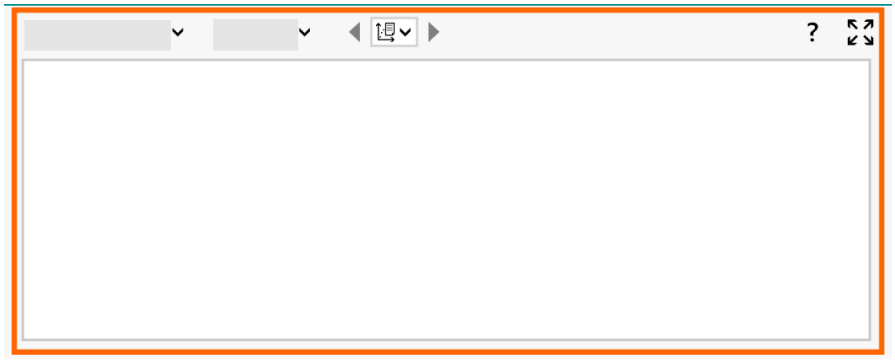
Example: The **New sample list** tab in the **Samples** work area



Area

Areas (**7**) are subelements of tabs. You can switch from one area to another by clicking on ⌄. The required subsection can be selected in an area.

Example: The **Curves and data** area with the opened **Live data** subsection

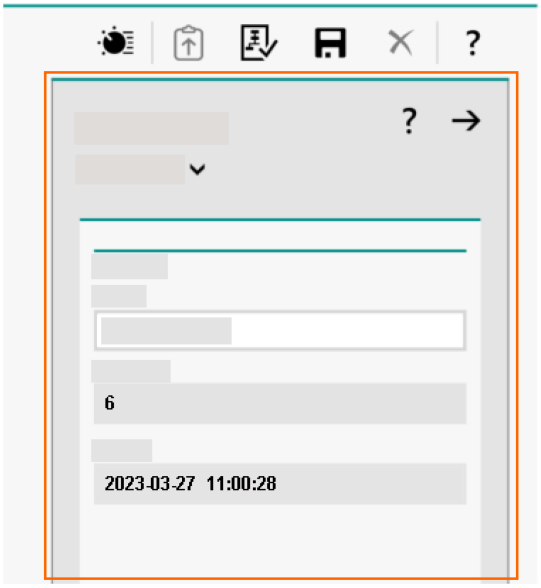


The size of the individual areas can be adapted using the horizontal and vertical divider (**6**) by pulling the areas in the desired direction while holding the mouse button pressed down.

Window

Windows are subelements of tabs or areas. These can be shown or hidden. The content of a window can be adapted with ⌄. The subsections that can be selected (e.g. **Parameters**) are displayed in the selection list.

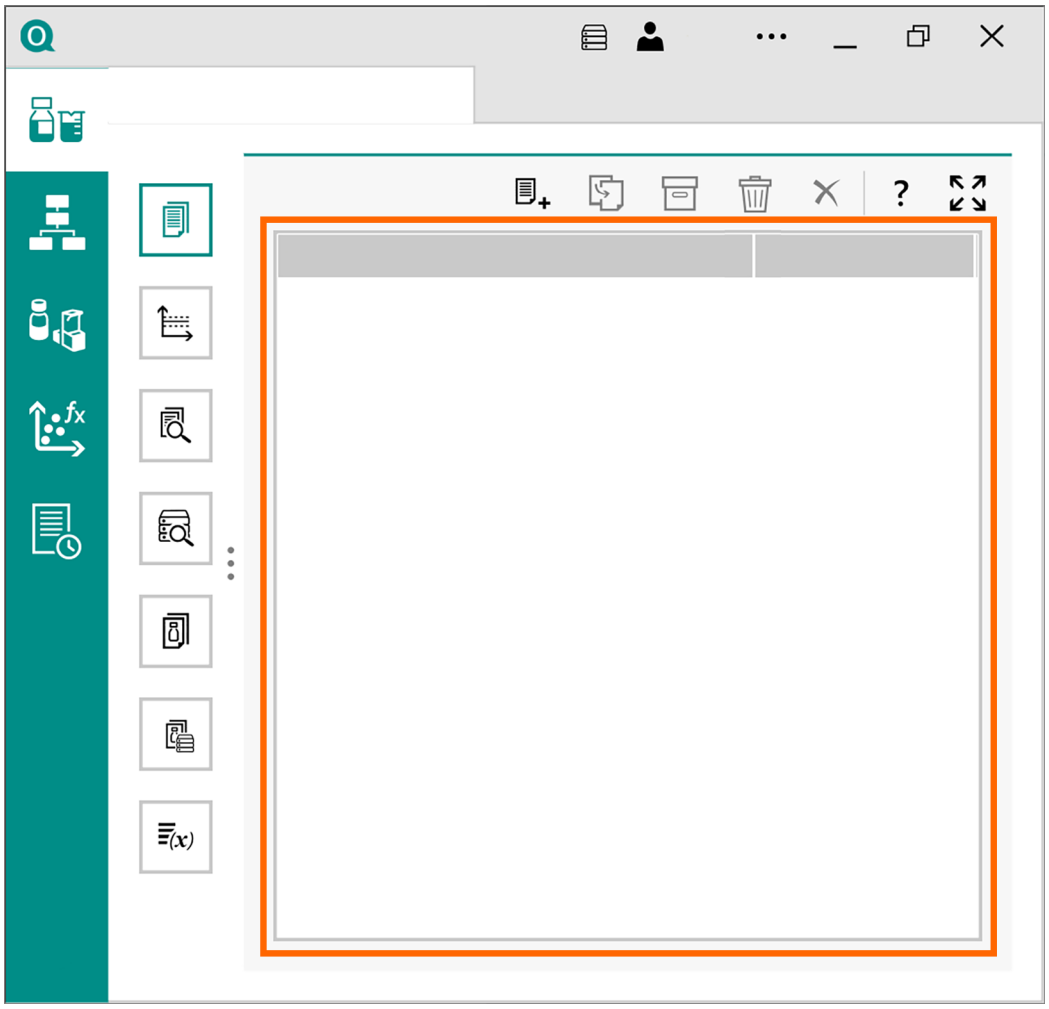
Example: The **Properties** window in the **New method** tab



Overview list

Every work area has subsections in which overview lists can be displayed (e.g. **Sample lists** in the **Samples** work area). All entries in overview lists open with a double-click.

Example:



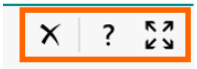
In each table, the entries of a column can be sorted by clicking with the left mouse button on the desired column head. A triangle on the left in the column head indicates the column according to which the current sorting has been performed and whether the entries are sorted in ascending or descending order.

Icons

Icons with which certain functions can be initiated or further areas can be opened are available not only for the title bar (**3**) but also for the toolbar (**7**). If the size of the database is critical, the title bar also displays information on the space used by the local database.

Example (3):

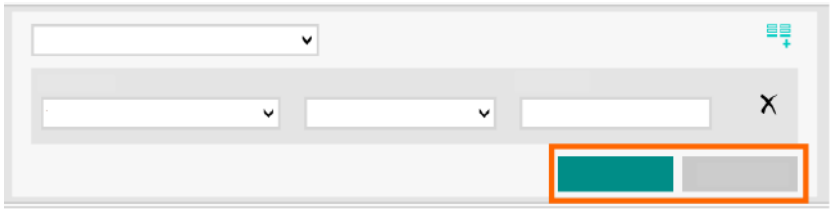
Example (7):



Buttons

Buttons are used to initiate actions and, unlike icons, they feature textual information on their functionality (e.g. **[Filter]**).

Example:



See also

Audit Trail – Actions (chapter 5.14, page 1171)

Equipment – Actions (chapter 5.12, page 851)

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

OMNIS Software – System overview (chapter 5.1, page 150)

Processes – Actions (chapter 5.11, page 378)

Samples – Definition (chapter 5.10.4, page 251)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

5.2.1 Library – Brief description

Libraries can be found in the following subsections in the OMNIS Software:

- **Processes ▶ Operating procedures**
- **Processes ▶ Methods**
- **Models ▶ Model hierarchies**

Clicking on opens the **Library** window. The following subsections can be selected here:

For operating procedures

- **Methods**
  Shows all saved methods.
- **Commands**
  Shows all commands which can be inserted into an operating procedure.

- **Optional runs**
  Shows the optional runs which can be inserted into an operating procedure.

For methods

- **Commands**
  Shows all commands which can be inserted into a method.
- **Optional runs**
  Shows the optional runs which can be inserted into a method.

For model hierarchies

- **Identification models**
  Shows all of the published identification models which can be inserted into a model hierarchy.
- **Quantification models**
  Shows all of the published quantification models which can be inserted into a model hierarchy.

Brief descriptions of the functions of the commands or of the optional runs can be found in the tooltips and more detailed information in the OMNIS Help

Search function

If the name of the required **method** is known, then it can be entered in the search field. In this case, only the methods are listed that contain the entered search terms in their name.

If the command type (e.g. **ADD**) or the name (e.g. **Add solution**) of the required **command** is known, it can be entered in the search field. In this case, only the commands are listed that contain the entered search terms in their command type or in their name.

If the name of the required **model** is known, then it can be entered in the search field. In this case, only the models of their respective category are listed that contain the entered search terms in their name.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Method – Definition (chapter 5.11.3, page 413)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

Operating procedure – Definition (chapter 5.11.1, page 379)

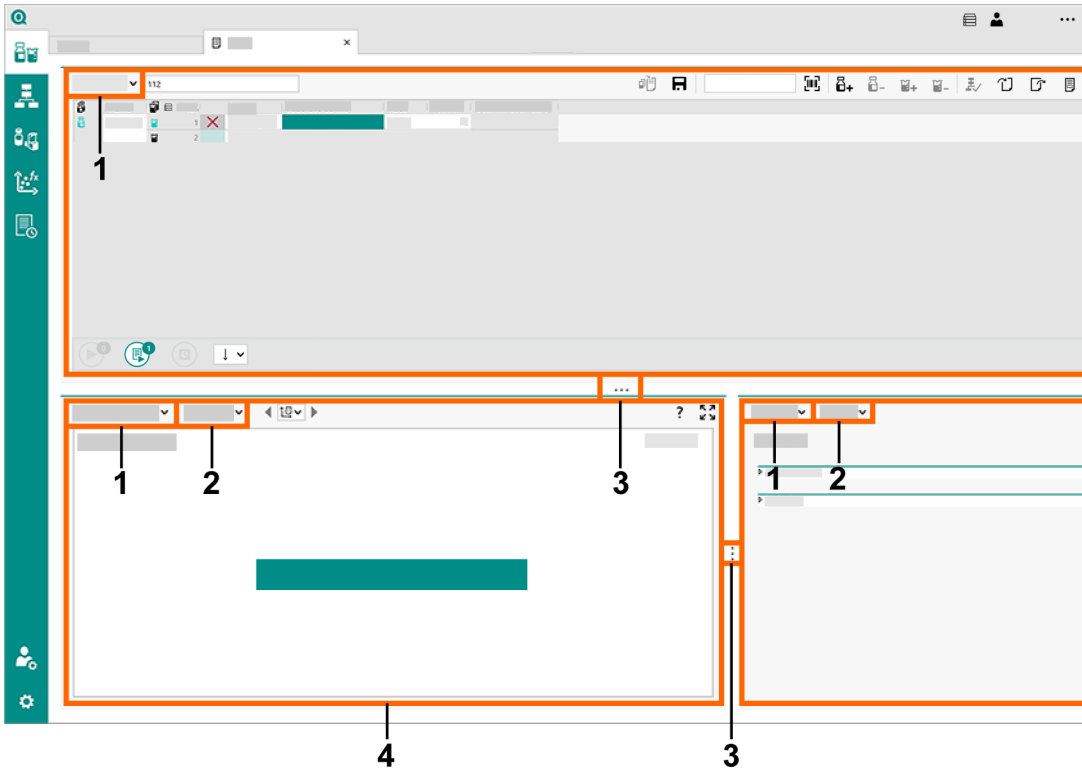
Run in case of a limit value violation – Definition (chapter 5.11.7, page 429)

Run in case of a stop – Definition (chapter 5.11.6, page 428)

Run in case of an error – Definition (chapter 5.11.5, page 427)

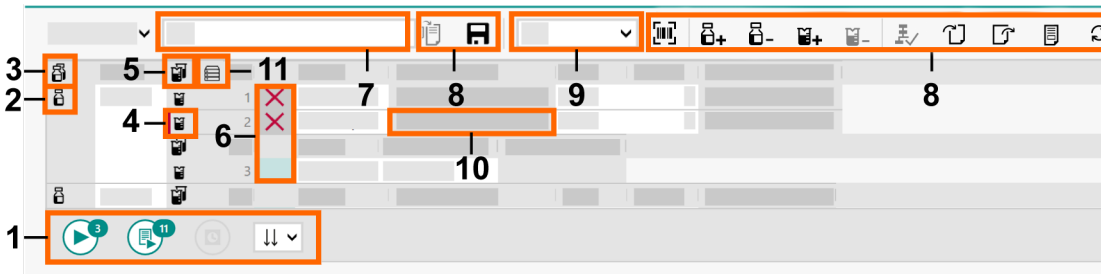
5.2.2 Sample list – Tab

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*



1	**Selecting an area** Selection from the areas **Sample list**, **Results**, **Curves and data** and **Subsample**.	**2**	**Selecting a subsection** Depending on the selected area, different subsections are available (see below).
3	**Divider** The size of the individual areas can be adjusted with the divider.	**4**	**Area** Display the selected area.

Sample list



1 **Managing determinations**
The determination can be started for the selected subsamples or for all executable subsamples in the sample list and at the same time the determination type can be selected (series determination or parallel determination). An ongoing determination can be stopped or paused.

2 **Sample and sample data**
A **sample** is marked in the sample list with the icon. A sample includes the sample data and the subsamples with their subsample data.

The **sample data** always includes a name for the sample. Additional sample data (e.g., analysis number, goods receipt date, batch number, etc.) can be defined with the help of a sample profile (template for sample data) or directly in the sample list. When a new sample is created, the sample data is inserted into the sample list from the selected sample profile. Sample data can be added directly to the sample list by right-clicking on the selected sample and selecting **Add sample data** in the context menu.

3 **Selecting all samples**

Click on to highlight all samples with the same sample data.

4 **Subsample and subsample data**

A **subsample** is marked in the sample list with the icon. A subsample is created from a sample in order to carry out an analysis.

The **subsample data** always includes a name for the subsample. Additional subsample data (e.g., sample size, dilution factor, etc.) can be defined in the operating procedure with which the subsample is analyzed. When a new subsample is created, the subsample data is inserted into the sample list from the selected operating procedure.

The status warning next to the icon indicates that errors have occurred during the run test, that results of the subsample are outside the defined limits or that there are model outliers. Additional information is displayed when the cursor is moved over the status warning. Additional information on the status warning: *(see "Subsamples – Statuses", chapter 5.10.7.3, page 276)*

5 **Selecting all subsamples**

Click on to highlight all subsamples with the same subsample data.

6 **Status of the subsample**

Subsamples can have different statuses. The background color of the status column shows the main status of a subsample. An additional icon displays the more detailed status of a subsample.

7 **Name field**

The name of the sample list can be modified here.

8 **Toolbar**

Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

9 Selecting a sample profile
A sample profile can be selected from the selection list.

10 Selecting an operating procedure
An operating procedure can be selected for the subsample from the selection list.

11 OMNIS Server
In the **OMNIS Client/Server system**, every subsample has an additional status that shows the status of the synchronization with the OMNIS Server.

Additional information on the synchronization status of subsamples in the **OMNIS Client/Server system**: *(see "Subsamples – Statuses", chapter 5.10.7.3, page 276)*

Results

- **Raw data**
  Raw data of a result (e.g. of an equivalence point) as well as determination data is displayed here.
- **Predictions**
  Here, results from predictions are displayed, post-evaluated and corrected.
- **Calculations**
  Calculation results are displayed and recalculated here.
- **Sample statistics**
  Statistics data for samples and subsamples are displayed here.
- **Monitoring**
  Results or variables which have activated result monitoring, including current value and limit value pairs, are displayed here.

Curves and data

- **Curves**
  Curves of ongoing and completed determinations are displayed here.
- **Measuring point lists**
  Measuring point lists of ongoing and completed determinations are displayed here.
- **Live data**
  Live data of ongoing determinations is displayed here.
- **Calibration curves**
  Calibration curves of executed calibrations or standard additions are displayed here.
- **Linear regression**
  The results of the regression analysis are displayed here as a straight line.

Subsample

During the determination, the OMNIS Software creates a protocol in the **Subsample** area that documents the entire analysis process. This protocol

is structured in several parts, which are presented respectively in the **Process**, **Equipment**, **History** and **Signatures** subsections:

- **Process**
  The subsample protocol for the operating procedure used and for the methods executed is displayed here.
- **Equipment**
  The subsample protocol for the work systems used and the corresponding functional units as well as the solutions and sensors used is displayed here.
- **History**
  Important data regarding sample, subsample, determination and history overview are recorded and displayed chronologically here.
- **Signatures**
  Signatures of subsamples are displayed here.

In the subsection **History**, click on **Show Audit Trail** to switch to the Audit Trail working area, where all entries related to the selected subsample are displayed.

See also

Displaying linear regression (chapter 5.10.12, page 344)

Displaying signatures (chapter 5.8.2, page 200)

Displaying the results (chapter 5.10.13, page 347)

Methods – Subsection (chapter 5.11.3.1, page 414)

Monitoring – Definition (chapter 5.10.13.4, page 355)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Predictions – Subsection (chapter 5.10.13.5, page 359)

Report template – Directory (chapter 5.10.1.4.1, page 233)

Reprocessing predictions (chapter 5.10.13.5.1, page 363)

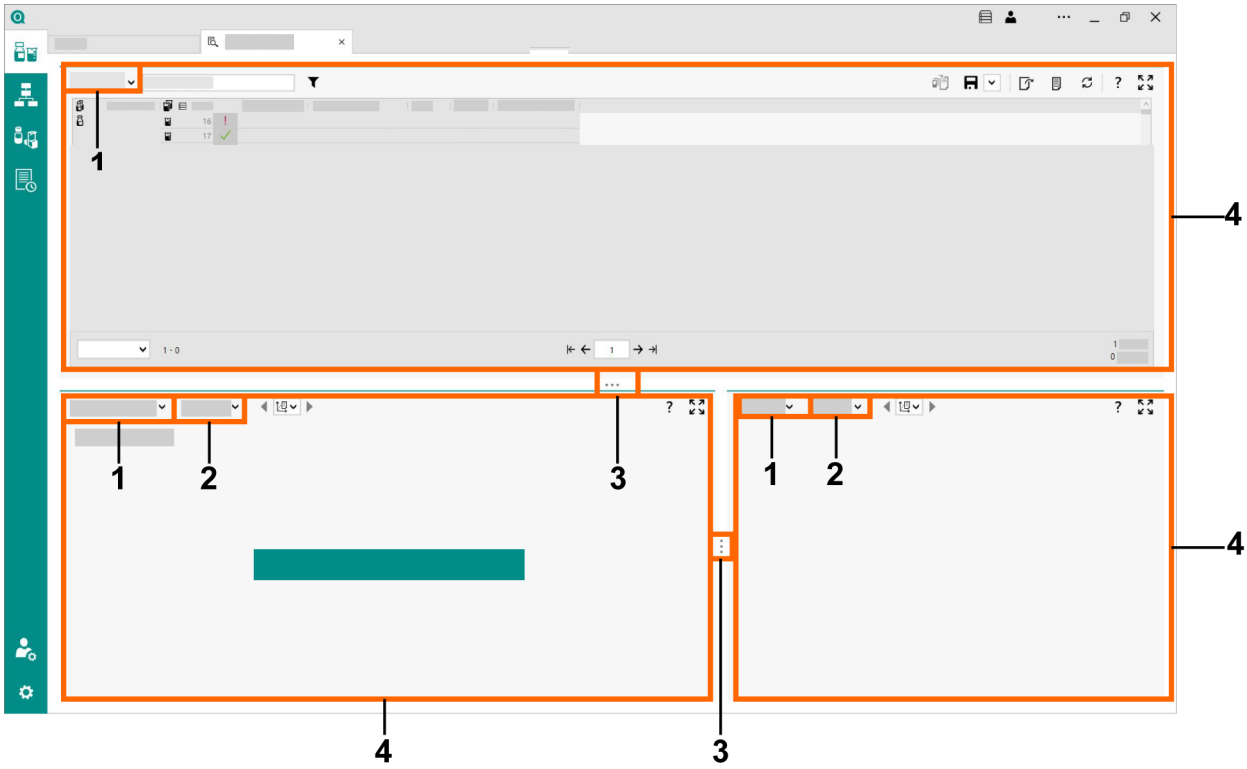
Restoring operating procedure and associated methods (chapter 5.11.1.9, page 402)

Sample lists – Subsection (chapter 5.10.1, page 210)

Signature – Brief description (chapter 5.8, page 197)

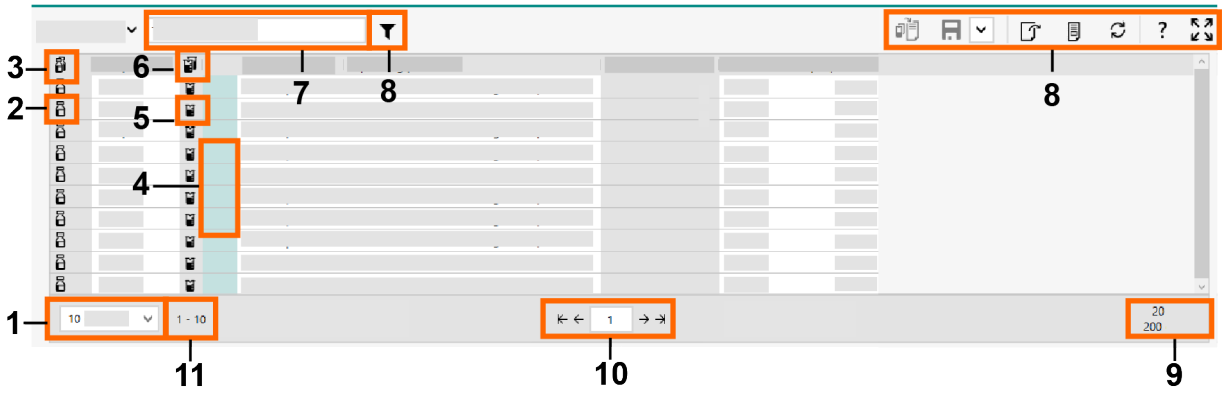
5.2.3 Search query – Tab

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*



1	**Selecting an area** Selection from the areas **Sample list**, **Results**, **Curves and data** and **Subsample**.	**2**	**Selecting a subsection** Different subsections are available, depending on the selected range.
3	**Divider** The size of the individual areas can be adjusted with the divider.	**4**	**Area** Display the selected area.

Search query



1 **Number of entries**
Selection of the number of entries that are to be displayed on a page.

2 **Sample and sample data**
A **sample** is marked in the sample list with the icon. A sample includes the sample data and the subsamples with their subsample data.

The **sample data** always includes a name for the sample. Additional sample data (e.g., analysis number, goods receipt date, batch number, etc.) can be defined with the help of a sample profile (template for sample data). When a new sample is created, the sample data is inserted into the sample list from the selected sample profile.

3 **Selecting all samples**
Click on to highlight all samples with the same sample data.

4 **Status of the subsample**
Subsamples can have different statuses. The background color of the status column shows the main status of a subsample. An additional icon displays the more detailed status of a subsample.

5 **Subsample and subsample data**
A **subsample** is marked in the sample list with the icon. A subsample is created from a sample in order to carry out an analysis.

The **subsample data** always includes a name for the subsample. Additional subsample data (e.g., sample size, dilution factor, etc.) can be defined in the operating procedure with which the subsample is analyzed. When a new subsample is created, the subsample data is inserted into the sample list from the selected operating procedure.

6 **Selecting all subsamples**
Click on to highlight all subsamples with the same subsample data.

7 **Name field**
The name of the search query can be modified here.

8 **Toolbar**
Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

9 **Number of pages and entries**
Total number of pages and entries in the search query.

10 **Current page**
Enter the desired page and click on **[Enter]** to confirm or click on ← or → to select either the next page or the previous page. Click on ↞ to display the first page or click on ↠ to display the last page of the list.

11 **Number of entries on the page**
Number of entries on the selected page.

See also

Creating Search queries and Server search queries (chapter 5.10.2.2, page 244)

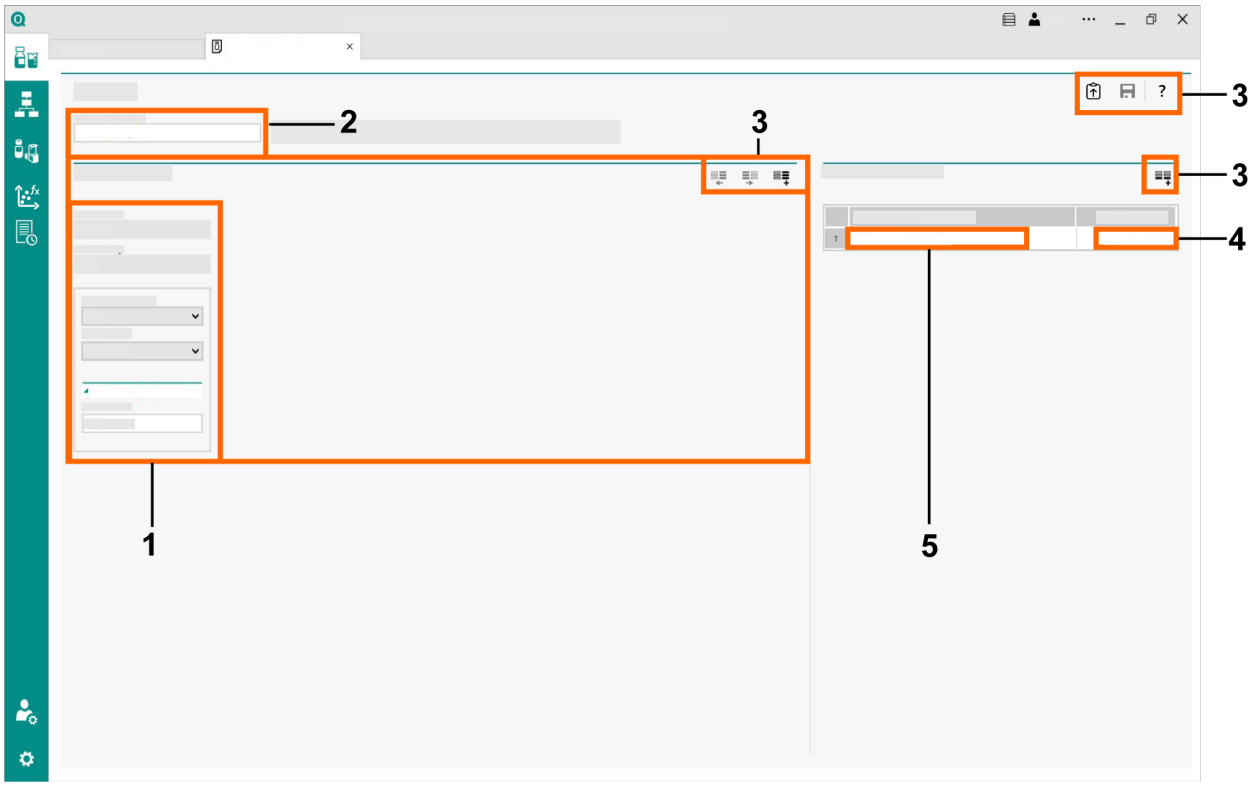
Filtering Search queries and Server search queries (chapter 5.10.2.3, page 246)

Sample list – Tab (chapter 5.2.2, page 159)

Subsamples – Definition (chapter 5.10.7, page 272)

5.2.4 Sample profile – Tab

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*



1	**Sample data** Define sample data that is available as sample identification.	**2**	**Name field** The name of the sample profile name can be modified here.
3	**Toolbar** Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*	**4**	**Enter number** Define the number of subsamples per sample to be created automatically when a sample is inserted into a sample list.
5	**Selecting an operating procedure** An operating procedure for the subsamples can be selected from the selection list.		

See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

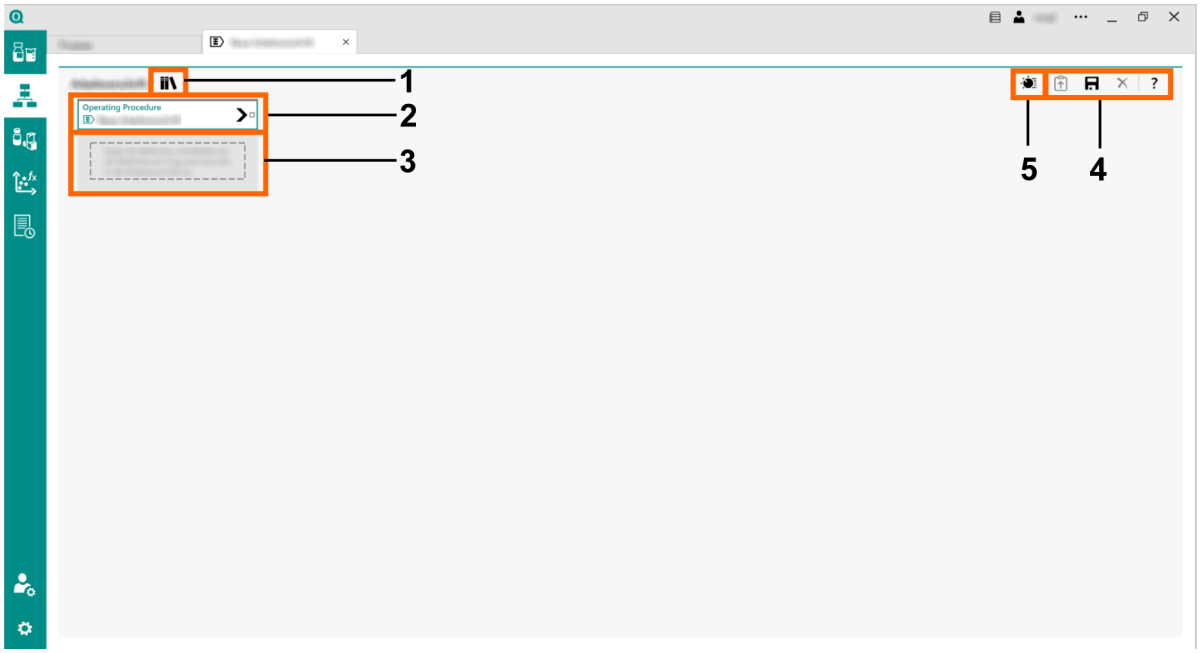
Operating procedure – Definition (chapter 5.11.1, page 379)

Sample profile – Definition (chapter 5.10.5, page 258)

5.2.5 Operating procedure and method – Tab

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Operating procedure



1 Library
Open a list with all available commands, methods and optional runs.

2 Define new operating procedure
Double-click on

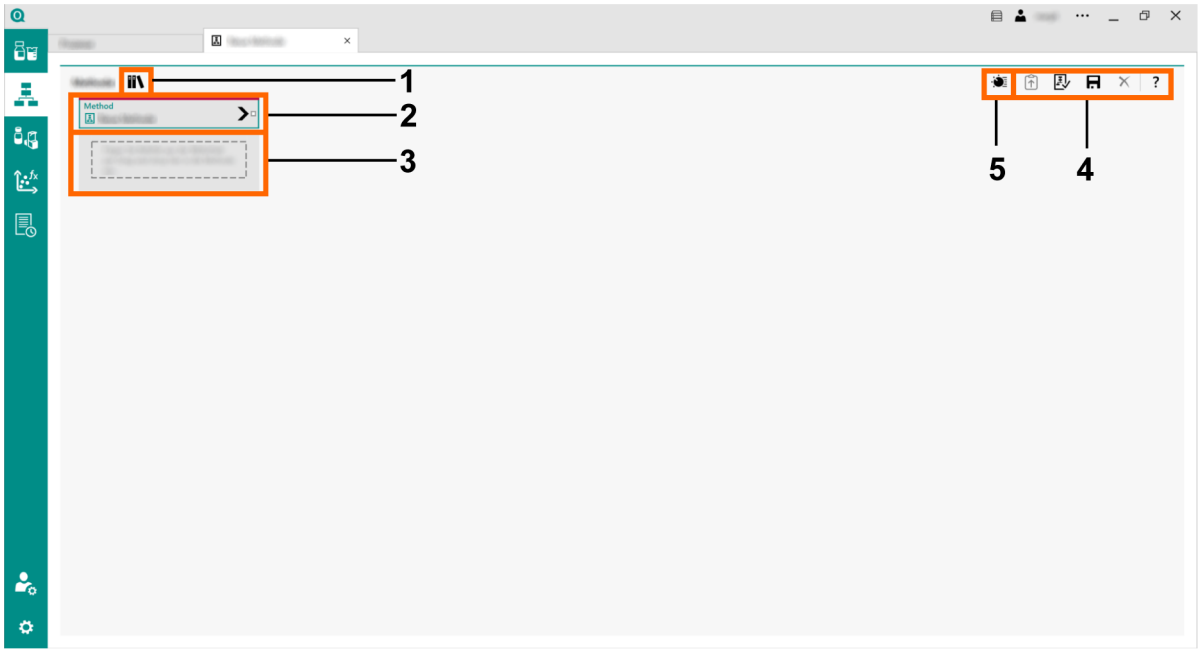
to directly open the **Properties** window in order to view or edit the properties of the selected element.

3 Compile new operating procedure
Use drag and drop to insert the desired elements from the library into the operating procedure.

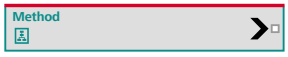
4 Toolbar
Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

5 Properties
Different functions and information are available from the subsections **General**, **Parameters**, **Execute with**, **Result monitoring**, **Reports**, **Exports** and **Web exports**, depending on the element selected.

Method



1 **Library**
Open a list with all available commands and optional runs.

2 **Define new method**
Double-click on 

to directly open the **Properties** window in order to view or edit the properties of the selected element.

3 **Compile new method**
Use drag and drop to insert the desired elements from the library into the method.

4 **Toolbar**
Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

5 **Properties**
Different functions and information are available from the subsections **General**, **Parameters** and **Execute with**, depending on the element selected.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Method – Definition (chapter 5.11.3, page 413)

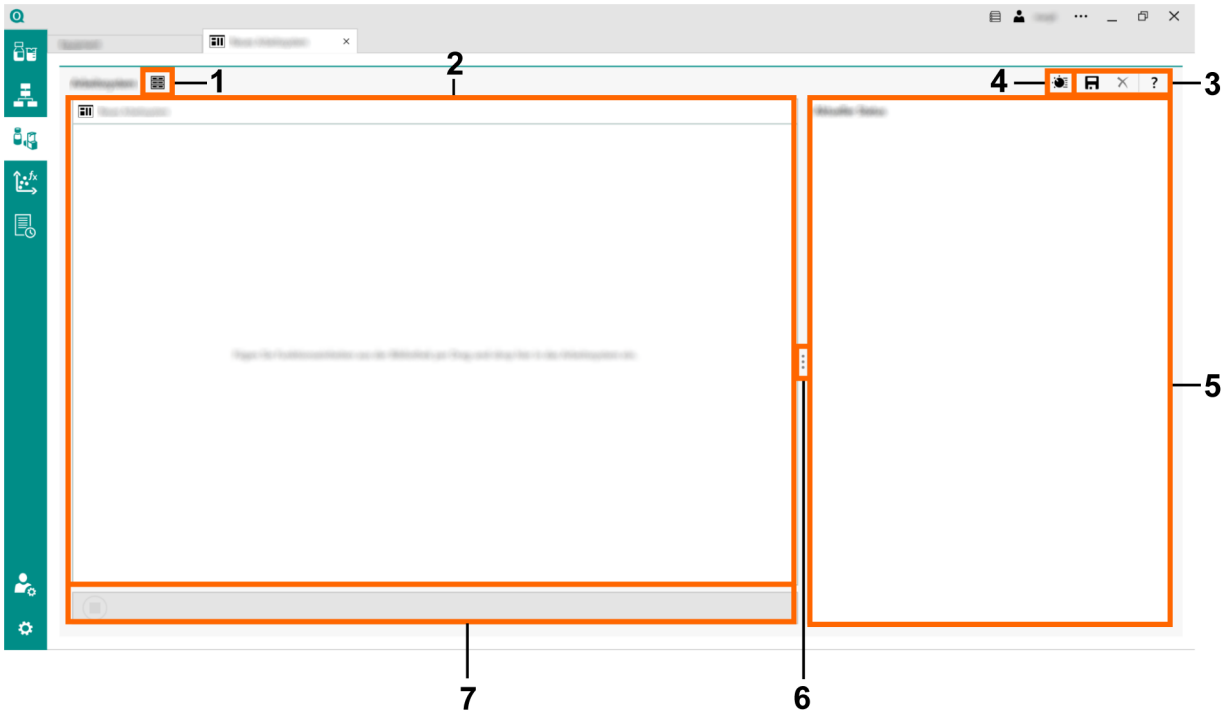
OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

5.2.6 Work system – Tab

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*



1	**Inventory** Open a list with all available functional units.
2	**Compile new work system** Use drag and drop to insert the desired functional units from the inventory into the work system.
3	**Toolbar** Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*
4	**Properties** Different functions and information are available in the subsection **General**, depending on the element selected.

5 **Current status**
The current status of the work system is displayed here. If the selected work system is currently being used for conditioning, for example, then the current measured values for the ongoing conditioning process will be displayed here.

6 **Divider**
The size of the individual areas can be adjusted with the divider.

7 **Stop functional units immediately**

Click on to immediately stop all functional units that are assigned to the highlighted work system. If a functional unit is still reserved by an ongoing determination, then it cannot be stopped.

See also

Creating a work system (chapter 5.12.4.4, page 989)

Functional unit – Definition (chapter 5.12.3, page 893)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Work system – Definition (chapter 5.12.4, page 987)

5.2.7 Sorting the overview list

All overview lists in the OMNIS Software can be sorted and formatted in any way you like.

Sorting and formatting

1 **Sorting individual columns**

- Click on a column title (**1**) to sort the overview list according to the selected column in either ascending or descending order.

2 Sorting several columns

- Sort multiple columns by clicking on one column title (**1**) while holding the **[SHIFT]** key pressed and then clicking on another column title (**2**).

The column title selected first determines the criterion to be used for sorting.

3 Adjusting the column width

- Position the mouse between the column titles (**3**), until the ⇔ icon appears.
- Holding the left mouse button pressed down, move to the left (decrease size of column) or the right (increase size of column).

See also

Audit Trail – Actions (chapter 5.14, page 1171)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Processes – Actions (chapter 5.11, page 378)

Samples – Actions (chapter 5.10, page 208)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

5.2.8 Copying table

Prerequisite:

- The **Samples** ▶ **Sample lists** subsection is opened. A table with data is displayed in the **Curves and data** or **Results** area.
  or
- The **Models** work area is open. A model, a slope/y-intercept correction or a model hierarchy is open and in the foreground. A table with data is displayed.

1 Copying table

- Right-click on the table to open the context menu and select **[Copy table]**.
  or
- Select the required lines and copy them using the **[CTRL]**+**[C]** key combination.

The table or the selected lines are copied to the clipboard.

2 Inserting table

- Open the required file in which the table is to be inserted.
- Insert the table into the file using the context menu or with the **[CTRL]**+**[V]** key combination.

5.3 OMNIS Software – Overview of functions

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

- *Functions with icons in the program as a whole*
- *Functions with icons in the Samples work area*
- *Functions with icons in the Processes work area*
- *Functions with icons in the Equipment work area*
- *Functions with icons in the Models work area*
- *Functions with icons in the Audit Trail work area*
- *Functions with icons in the User management work area*
- *Functions with key combinations in the program as a whole*
- *Functions with mouse clicks in the program as a whole*

Functions with icons in the program as a whole

OMNIS Server

Information on the status display of the OMNIS Server: **OMNIS Server connected**, **OMNIS Server not connected**, **Connecting to the OMNIS Server**, **OMNIS Server not compatible** and **Differently configured operation modes**

Note: Applicable only in the **OMNIS Client/Server system**.

C1-PV

Operation mode

DQ-FS

Information if the OMNIS system is running in a special operation mode for service activities.

Additional information on the operation mode: *(see "Operation mode – Definition", chapter 6.1.7, page 1233)*

Critical database size almost reached

Information on the space used if the critical database size of the local database is almost reached.

Note: Is only displayed if the space used by the local database is larger than or equal to 8 GB.

Critical database size reached

Information on the space used if the size of the local database is critical.

Note: Is only displayed if the space used by the local database is larger than or equal to 9 GB.

Logged in user

Display the currently logged-in user in the tooltip.

Additional functions: **Lock OMNIS Software**, **Change password**

Missing assignment of data permissions

Information for the user currently logged in announcing that data permission assignments are missing.

Tools

Further information on and functions for the OMNIS Software.

Further functions: **OMNIS Help**, **About OMNIS Software**, **Collect OMNIS system information** or **Send OMNIS environment information**.

Open the help

Open OMNIS Help.

Minimize

Minimize the program window.

Restore down

Reduce the program window down to the size defined prior to maximization.

Maximize

Maximize the program window to the full monitor size.

Close

Close the program window.

Close area

Close the area.

Maximize

Maximize the subsection.

	Minimize Minimize the subsection.
	Save Save all changes.
	Delete Delete the selected object.
	Update view Reload the view or list. All entries are reloaded. If there are unsaved changes or disconnected instruments, then these will be discarded.
	Properties Open the **Properties** window to display and edit the settings of the currently selected object.
	Open selection list Expand the selection list with various options for the field.
	Import Import the selected object.
	Export Export the selected object. **Audit Trail:** All entries that match the currently applied filter criteria are exported as a CSV file to the target folder. Files for the integrity check of this CSV file are also created in the target folder.
	Duplicate Duplicate the selected object.
	Archive **Samples:** The samples in the selected sample list are archived along with their subsamples. They are deleted from the database. The sample list will also be deleted. **Audit Trail:** All entries are archived as a CSV file, saved to the target folder and deleted from the current database. Files for the integrity check of this CSV file are also created in the target folder.
	Create report Create the report for the selected object manually.

	Open or close filter criteria Open or close the area for selecting configurable filter criteria.
	Add input field Add a new column to the right with input fields for data.
	Delete input field Delete the selected input field.
	Move input field to the left Move the selected column to the left by 1 position.
	Move input field to the right Move the selected column to the right by 1 position.
	Add new row Add a new row below, e.g. for another filter criterion.
	Move row up Move the selected row up by 1 position.
	Move row down Move the selected row down by 1 position.
f_x	**Formula editor** Open the **Formula editor** window to enter formulas.
(x)	**Variable selection** Open the **Variables** window for selecting the required variable.

Functions with icons in the Samples work area

	Create sample list Create a new sample list in which samples and subsamples can be inserted, edited and managed.
	Create search query Create a new search query in which you can search for samples and subsamples using filter criteria. The results can be saved as sample list or search query for later use.

Create server search query

Search for samples and subsamples on the OMNIS Server using configurable filter criteria. The results can be saved as a server search query or transferred to a new sample list.

Note: Applicable only in the **OMNIS Client/Server system**.

Remove sample list from local OMNIS Client

Remove the samples in the sample list along with their subsamples from the local system. The samples and subsamples are retained on the OMNIS Server.

Remove the sample profile from the local OMNIS Client

Remove the selected sample profile from local system. A published sample profile is removed only from the local OMNIS Client and is retained on the OMNIS Server. Existing samples that were previously recorded with this sample profile are retained in the database.

Note: Applicable only in the **OMNIS Client/Server system**.

Create sample profile

Create a new sample profile to facilitate the entry of recurrent sample data.

Delete sample profiles

Delete the selected sample profiles. Existing samples that have previously been entered with the sample profiles are retained in the database.

Note: Applicable only in **OMNIS Stand-Alone**.

Delete server sample profiles

Delete the selected server sample profiles from the OMNIS Server. The associated sample data is not deleted when the server sample profile is deleted. The deleted sample profile is retained locally on the OMNIS Clients that downloaded the server sample profile before it was deleted.

Note: Applicable only in the **OMNIS Client/Server system**.

Download sample profile

Download the sample profile and associated sample data. The downloaded sample profile is displayed in the **Sample profiles** subsection and can be used.

Note: Applicable only in the **OMNIS Client/Server system**.

Create system variable

Create a new system variable for use throughout all commands, methods and operating procedures.

Functions with icons in the Sample lists, Control charts, Search queries, Server search queries and Sample profiles subsection

More saving options

Select from the following options for saving the results of a local search query:

- Select the **Save as new search query** option to save the configured filter criteria as a new search query.
- Select the **Save as new sample list** option to save the samples and subsamples that have been found with the configured filter criteria as a new sample list.

Select from the following options for saving the results of a server search query:

- Select the **Save as new server search query** option to save the configured filter criteria as a new server search query.

Next or previous page

Display the next or previous page.

First or last page

Display the first or last page.

Add subsamples to a new sample list

Add the highlighted subsamples to a new sample list. The subsamples remain in the original sample list.

In the **OMNIS Client/Server system**, the subsamples are thus downloaded to the OMNIS Client.

Adding samples based on the sample profile IDs

Add the samples contained in the sample profile to the sample list.

Add a sample

Add a new sample to the sample list.

Remove sample

Remove the selected sample from the current sample list. The sample is retained in the database.

Add a subsample

Add a new subsample to the selected sample.

Remove subsample

Remove the selected subsample from the current sample list. The subsample is retained in the database.

Perform manual run test

Check the fulfillment of all conditions for successful execution of the subsamples.

Restore operating procedure or methods

Restore the operating procedure or methods to the version they were in at the time the subsample was executed.

Start selected determinations

The selected and executable subsamples are analyzed. The number of the selected and executable subsamples is indicated on the button.

Start list

All executable subsamples in the sample list are analyzed. The number of the executable subsamples is indicated on the button.

Stop determination immediately

All running determinations are canceled.

Stop determination after a delay

The running determination of the subsample is run until completion. Other determinations are not restarted.

Series determination

Analyze the subsamples sequentially.

Parallel determination

Analyze the subsamples simultaneously.

Restore focus

The focus on the currently running subsample is restored.

Add subsamples to sample series

All executable subsamples in the sample list are added to the running sample series and they are then analyzed. The number of subsamples is indicated on the button.

Add to running sample series

The selected subsample is added to the running sample series and analyzed.

Remove from running sample series

The selected subsample is removed from the sample series currently running.

Reset to status "Ready"

The selected, canceled subsample is reset to "Ready" status and can be analyzed once again.

Hold determination

The running determination of the subsample is paused.

Stop determination

The running determination of the subsample is stopped.

Select command

Select the command for which the curve is to be displayed.

Select command

Select the command for which the live data, measuring point list or raw data is to be displayed.

Overlay curves

Overlay the curves of several subsamples.

Reevaluate curves

Reevaluate the curve of the subsample.

Recalculate results

Recalculate the results of the subsample.

Reevaluate results

Reevaluate the results of the subsample.

Publish sample profile

Publish the sample profile and associated sample data. In order to publish a sample profile, all associated operating procedures must also be published. The published sample profile is available to all connected OMNIS Clients.

Note: Applicable only in the **OMNIS Client/Server system**.

Create control chart

Create a new control chart in which statistical samples from selected sample lists are entered in relation to a user-defined variable.

Edit control chart

Edit the parameters of an open control chart.

Functions with icons in the Processes work area

Create operating procedure

Create a new operating procedure in which methods and commands can be inserted and edited.

Create method

Create a new method in which commands can be inserted and edited.

Delete operating procedures or methods

Delete all selected operating procedures or methods. When operating procedures are deleted, the methods they contain are retained in the database.

Signed operating procedures or methods are locked and cannot be deleted.

Delete server operating procedures or server methods

Delete all selected server operating procedures or server methods from the OMNIS Server. To be able to delete a server method/server operating procedure, it must first be withdrawn.

Note: Applicable only in the **OMNIS Client/Server system**.

Remove operating procedures or methods from the local OMNIS Client

Remove the selected operating procedures or methods from the local system. Published operating procedures or methods are removed only from the local OMNIS Client and are retained on the OMNIS Server.

Note: Applicable only in the **OMNIS Client/Server system**.

Download operating procedure or method

Download the operating procedure or method. When downloading, the associated processes or work systems, respectively, are also downloaded.

Note: Applicable only in the **OMNIS Client/Server system**.

Functions with icons in the Operating procedures or Methods subsection

Library

Open the **Library** window with the list of all available elements that can be inserted into operating procedures and methods.

Add report definition or export definition

Add a report definition or an export definition.

Remove report definition or export definition

Remove the defined report definition or export definition.

Validate method

Check the assignments of functional units and work systems for correctness.

Publish operating procedure or method

Publish the operating procedure or method and the associated processes or work systems, respectively. They are thus available for all connected OMNIS Clients and are protected against changes.

Note: Applicable only in the **OMNIS Client/Server system**.

Withdraw operating procedure or method

Withdraw the operating procedure or method. The utilization of the withdrawn operating procedures or methods is limited. The utilization of operating procedures that include the withdrawn method is also restricted when a method is withdrawn.

Note: Applicable only in the **OMNIS Client/Server system**.

Functions with icons in the Equipment work area

Inventory

Open the **Inventory** window to select and insert instruments, functional units, analog sensors and conductivity standards for solutions.

Add instrument manually

Add instruments from other subnets to the **Inventory** window.

Remove added instrument (in the **Inventory** window)

Remove the instrument added from the **Inventory** window. Work systems which were created with this instrument are retained.

Manual control

Open the **Manual control** window for the manual control of instruments and functional units.

Assemble work systems

Assemble a work system of functional units for executing a method.

Define advance warning time

Define the advance warning time for the expiry date of sensors, solutions and titers.

Create a new temperature table

Create a new temperature table for a custom pH calibration buffer.

Functions with icons in the Models work area

	Create quantification model Create a new quantification model for the calculation of a reference parameter.
	Creating the slope/y-intercept correction Create a new slope/y-intercept correction for the correction of the selected quantification model.
	Create identification model Create new identification model to identify samples.
	Create a model hierarchy Create a new model hierarchy to link models.
	Publish Publish the quantification model or the slope/y-intercept correction to be able to use it in determinations and repredictions. Publish the identification model or model hierarchy so that it can be used in determinations.
	Edit reference parameter Edit the reference parameter of the quantification model.
	Automatic splitting of dataset Split the dataset automatically into calibration dataset, validation dataset and outlier dataset.
	Add spectra Add spectra to the quantification model or identification model. Opens the dialog for selecting spectra from a sample list or search query.
	Remove spectra Remove spectra from the quantification model or identification model.

Functions with icons in the Audit Trail work area

	Check integrity All Audit Trail entries are checked for completeness and integrity. A report on the integrity errors can be exported as a CSV file.

	Display process overview The process overview of the selected Audit Trail entry opens. Displays the process sequence at the time of an action performed by the user on an operating procedure or method.

Functions with icons in the User management work area

	Create user Create a new user for which user data can be defined and edited.
	Create user group Create a new user group to which users can be assigned. During the assignment, the user is given the corresponding roles and permissions of the user group.
	Create a user role Create a new user role that can be assigned to a user group. Different permissions can be selected for the user role.

If the user management with Active Directory integration has been activated, no users can be created and edited in the OMNIS Software. New user accounts can be created and edited via Active Directory outside of the OMNIS Software and are added automatically to the OMNIS Software during restart.

Functions with key combinations in the program as a whole

Functions with key combinations in the **Sample list** tab: *(see "Sample list – Overview of functions", chapter 5.10.1.5, page 240)*

[F1]	**Open the help** Open OMNIS Help.
[F5]	**Update view** Reload the view or list. All entries are reloaded. If there are unsaved changes, then these will be discarded.
[CTRL]+[L]	**Lock OMNIS Software** Lock the OMNIS Software.
[CTRL]+[S]	**Save** Save all changes.

[CTRL]+[D]	**Duplicate** Duplicate the selected object.
[CTRL]+[ENTER]	**Continue** Confirm the entered data and close the input dialog of the REQUEST command.
[CTRL]+[X]	**Cut** Cut and copy selected object to clipboard.
[CTRL]+[C]	**Copy** Copy selected object to clipboard.
[CTRL]+[V]	**Paste** Paste the object from the clipboard at the selected position.
[CTRL]+[I]	**Create or add** Create or add a new system variable.
[DELETE]	**Remove or delete** Remove (samples and subsamples) or delete (all other objects) selected object from the current display.
[CTRL]+[DELETE]	**Delete** Delete selected object (sample or subsample) permanently from the database.
[CTRL]+[Z]	**Undo** Undoes the last entry in the input field.
[CTRL]+[Y]	**Repeat** Repeat the last entry in the input field after it was previously undone.

Functions with mouse clicks in the program as a whole

Functions with mouse clicks in the tab **Sample list**: *(see "Sample list – Overview of functions", chapter 5.10.1.5, page 240)*

Left mouse click	**Select an object** Select the object.

Mouse click	**Close tab** Close a tab. The cursor must be positioned on the tab that is to be closed.
Right mouse-click	**Open context menu** Open context menu with functions for the selected object.
Drag and drop	**Insert and move elements** Insert available elements from the **Inventory** or **Library** window and move them to the desired position. Move active tabs to the desired position.
Double-click	**Open context-dependent windows** ▪ In the **Instruments** subsection, the **Manual control** window is opened. ▪ In the **Sensors** subsection, the **Properties** window with the **Specific data** area is opened. ▪ In the **Method** and **Operating procedure** tabs, double-clicking on the operating procedure or method opens the **Properties** window with the **Parameters** area. ▪ Opens a new tab with the selected object in the overviews of the **Processes**, **Samples** and **Equipment** work areas. **Open an input field** ▪ An input field is opened in the **Processes** work area and **Quantification models** subsection in the overview lists in the **Tags** column. **Mark entire word** Within a text input field, mark the selected word.
Click 3x	**Mark entire line** Within a text input field, mark the selected line up to the next line. Mark the selected variable in the **CALL WEB API** command under **[Edit Request Body]**.

See also

Data permissions – Definition (chapter 4.5.9, page 105)

Methods – Subsection (chapter 5.11.3.1, page 414)

Models – Actions (chapter 5.13, page 1054)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Server – Status (chapter 4.1.1, page 21)

Operating procedure and method – Tab (chapter 5.2.5, page 168)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Operation mode – Definition (chapter 6.1.7, page 1233)

Sample list – Tab (chapter 5.2.2, page 159)

Sample profile – Tab (chapter 5.2.4, page 166)

Sample profiles – Subsection (chapter 5.10.5.1, page 259)

Search query – Tab (chapter 5.2.3, page 164)

Server methods – Subsection (chapter 5.11.4.1, page 426)

Server operating procedures – Subsection (chapter 5.11.2.1, page 412)

Work system – Tab (chapter 5.2.6, page 170)

5.4 Locking or unlocking the OMNIS Software

The OMNIS Software can be locked manually or automatically and thus protected against changes to the data.

Information on the behavior of processes in OMNIS Software during login and logout: *(see "OMNIS Software – Login/logout", chapter 5.5, page 190)*

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Locking the OMNIS Software manually

1 Locking manually

- After clicking on in the title bar of the OMNIS Software, select the **[Lock OMNIS Software]** function in the selection list.
- Alternatively, lock the OMNIS Software with **[CTRL + L]**.

Locking the OMNIS Software automatically

1 Activating automatic locking

- Enable the check box **Automatic locking** in **User management ► User management settings** and enter the required time.

2 Saving the settings

- Click on to save the settings.

If no user activity (e.g. use of the keyboard or the mouse) is carried out, the OMNIS Software is locked after the time has elapsed.

Unlocking the OMNIS Software

1 By the same user

- Enter the password in the **Unlock OMNIS Software** dialog.
- Click on **[Unlock]** to unlock the OMNIS Software.

2 By another user

- Click on **[Switch user]** in the **Unlock OMNIS Software** dialog.
- In the **Log in to OMNIS Software** dialog, enter the **User ID** and the **Password** and click on **[Login]**.
- Clicking on **[Cancel]** in the **Log in to OMNIS Software** dialog, returns the user to the **Unlock OMNIS Software** dialog, where the previously logged-in user can unlock the OMNIS Software.

The following is to be observed in the event of a login by another user:

- During ongoing processes that the user has not completed yet, such as importing data or pending prompts for confirmation, no new user can log in. The user has to first finish the started processes before another user is able to log in.
- Unsaved changes made by the previously logged in user are discarded at the time of a new login.
- The only views that will be loaded are those for which the newly logged in user has the required rights.
- If the **Audit Trail** function is enabled, then the change of user will be recorded in the Audit Trail. All changes up to the unlocking are assigned to the previously logged in user. All changes by the newly logged in user after the change of user are assigned to this user.

See also

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User groups – Definition (chapter 4.5.6.1, page 81)

User groups – Properties (chapter 4.5.6.2, page 82)

User interface OMNIS Software – Overview (chapter 5.2, page 151)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

User roles – Directory (chapter 4.5.7.3, page 88)

User roles – Properties (chapter 4.5.7.2, page 87)

5.5 OMNIS Software – Login/logout

Some processes that are started when using the OMNIS Software are continued in the background by the Metrohm **Miami LabLogic** service after closing the OMNIS Software or a tab or after a change of user on the Windows desktop. Seamless transition, e.g. in the event of a shift change, is possible. When logging into the OMNIS Software again, any error messages that have occurred in the meantime are displayed to the next user at startup. These error messages may be discarded or confirmed only by a user with the necessary user rights.

A user without the corresponding user role can also log into OMNIS, but can perform only the activities that have been released for him.

This functionality is particularly relevant in the following use cases:

- **Change of user:** The user currently logged on may log out without canceling the operation of a process. This allows another user to log on to the same computer afterwards.
- **Close the OMNIS Software:** The OMNIS Software may be closed at any time without interrupting the process run.
- **Close the tab:** The tab with the running determination may be closed at any time without canceling the process run.

The process is canceled when the **Metrohm Miami LabLogic** service is stopped (e.g., when the computer is switched off or restarted). These processes are discarded and may need to be restarted manually in the OMNIS Software.

For the behavior of importing, exporting and creating a report with a change of user in the OMNIS Software: *(see "Locking or unlocking the OMNIS Software", chapter 5.4, page 188)*

Metrohm OMNIS Printing is installed by default as an application, which means that print orders are canceled after signing out of Windows. If print orders are to be continued after signing out of Windows, then Metrohm OMNIS Printing must be configured as a service. Additional information:

Determinations

The sequence of running determinations can be tracked by restarting the OMNIS Software or by reopening the tab. If one or more of these determinations have been completed, then the results are available in the OMNIS Software. This information is displayed in **Samples** ▶ **Sample lists** ▶ **Sample list**. If an error occurred during the process, then the message will be displayed at the next login.

The newly logged-in user must have the necessary user rights to display the sequence or results of these determinations. The sequence of running determinations continues, regardless of the user rights assigned to the newly logged-in user.

Use cases

The following examples show how to use the new functionality. The following prerequisites apply here:

User A has the user role of a **laboratory manager**.

User B has the user role of a **routine user**.

Changing the user in the OMNIS Software while the determination is running:

1. User A closes the OMNIS Software.
2. User A logs off from the Windows operating system.
3. User B logs into the operating system with his Windows user account.
4. User B logs on to the OMNIS Software with his user account.

User B is now able to make full use of the OMNIS functionalities that have been enabled for him, without affecting the determination of user A. Any error messages that occur are also saved and cannot be removed by user B by clicking **[OK]**, as he does not have the corresponding release.

Resuming work after logging out of the Windows operating system and the OMNIS Software:

1. User A has a running determination in the OMNIS Software.
2. User A closes the OMNIS Software and logs out of the Windows operating system.
3. User B logs into the Windows operating system and the OMNIS Software with his respective user accounts.
4. User B performs the work that has been released for him.

5. User B closes the OMNIS Software and logs out of the Windows operating system.
6. User A logs on to the Windows operating system and the OMNIS Software with his respective user accounts.

If the determination was completed during user A's absence, then user A has access to the results. Otherwise, user A can retrieve and track the current progress. If any errors occurred during the determination, then they are now displayed to user A.

See also

Creating report (chapter 5.10.1.4, page 224)

Data permissions – Definition (chapter 4.5.9, page 105)

Determination – Definition (chapter 5.10.8, page 295)

Determination – Preparation and follow-up (chapter 5.10.8.10, page 313)

Locking or unlocking the OMNIS Software (chapter 5.4, page 188)

Preparing determination (chapter 5.10.8.9, page 310)

Report template – Directory (chapter 5.10.1.4.1, page 233)

Starting determination (chapter 5.10.8.6, page 304)

Stopping a determination (chapter 5.10.8.7, page 308)

User rights – Directory (chapter 4.5.7.4, page 89)

5.6 Modification comment – Brief description

Information on the settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

If the **Modification comment** function is activated in **Settings ► Advanced settings**, under the option **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11**, then the **Modification comment** dialog will appear before saving the sample list.

The dialog appears only for content changes to the sample list that affect the database (e.g. adding, deleting, renaming samples and subsamples).

The dialog does not appear for changes that only affect the composition of the sample list (e.g. renaming the sample list or removing, cutting or blocking samples).

Before the modifications can be saved, a reason for the modification must be selected. An optional modification comment can be entered.

Modification comment dialog

Reason for modification	Selection of defined default reasons, e.g. ▪ Carried out reevaluation ▪ Carried out recalculation ▪ Modified
Modification comment	Optional entry of a change comment that is saved in addition to the reason for the change.

See also

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

5.7 Enabling monitoring

- *Enable monitoring*
- *Define advance warning time*
- *Carrying out a determination after the expiry date is reached*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

Enabling monitoring

The **Enable monitoring** function is possible for the following equipment:
- Sensors
- Calibration for sensors of the types ion-selective electrode, conductivity measuring cell and ph electrode
- Solutions
- Titer

1 Opening a subsection

- For monitoring the **expiry date** of sensors or calibrations, open the **Equipment** ► **Sensors** subsection.

- For monitoring the **expiry date** of solutions or titers, open the **Equipment** ▶ **Solutions** subsection.

2 Opening specific data

- Click to select the required equipment.
- Click on to open the **Properties** window.
- In **Properties**, open the **Specific data** subsection.

3 Opening a parameter group

- For monitoring the **expiry date** of sensors, open the **Sensor data** parameter group.
- For monitoring the **expiry date** of calibrations, open the **Calibration data** parameter group.
- For monitoring the **expiry date** of solutions, open the **Solution data** parameter group.
- For monitoring the **expiry date** of titers, open the **Titer data** parameter group.

4 Enter the working life or validity period

- For sensors and solutions under **Working life**, enter the duration in days or define by clicking on .
- For calibrations and titers, enter the duration in hours under **Validity period**.

5 Enabling monitoring

- Enable the **Enable monitoring** function by clicking on the check box.

As soon as monitoring is enabled, the monitoring status is displayed in the respective column in the overview list.

Additional information on the status of equipment:

- *(see "Sensor – Status", chapter 5.12.6.3, page 1007)*
- *(see "Solution – Status", chapter 5.12.7.3, page 1019)*

6 Saving changes

- Save changes by clicking on .

- Modified data of equipment cannot be saved as long as the equipment is being used in an ongoing determination.
- The basis for the calculation of the expiry date or time interval are the date and time settings of the operating system used, i.e. time zones, daylight savings time and leap years are taken into account.
- If the date and time settings are changed, then the expiry dates, calibration data, adsorber data and working life initially entered will not be changed. This data is saved on the equipment as well as in the database.

Defining the Advance warning time

The **Define advance warning time** function is possible for the following equipment:

- Sensors
- Solutions
- Titer (optional)

Prerequisite:

- For sensors, the **Sensors** overview list is open.
- The **Solutions** overview list is open for solutions or titer.

1 Opening the Advance warning time window

- Click on to open the **Advance warning time** window.

2 Selecting the advance warning time

- Select the **Enter value** option from the selection list in **Advance warning time** for every equipment type that is to be monitored. For the defined advance warning time to take effect, the *Activate monitoring* function must be enabled for at least one piece of equipment of the respective type.
- Enter the required **Advance warning time** in days.

If no advance warning time is to be defined, then the **No advance warning** option must be selected in the selection list.

3 Saving changes

- Save all changes by clicking on .

A warning message appears once the time for which the advance warning has been set is reached. The time for the first warning is

defined as the **Expiry date** minus the **Advance warning time** in days.

Carrying out a determination after the expiry date is reached

If a determination is started with expired equipment, then a warning message will appear. To execute the determination, the following options are available:

- *Cancel and restart determination*
- *Continue determination*

Canceling and restarting the determination

Prerequisite:

- A determination was started in the Sample list.
- Before the subsample determination, the **Expiry date exceeded** warning message is displayed.

1 Canceling the determination

- Click on **[Cancel]** in the warning message to cancel the execution of the subsample.
- Replace the equipment.

The status of the subsample is reset to **Ready** automatically.

2 Restarting the determination

- Restart the subsample determination by clicking on ▶.

Continuing the determination

Prerequisite:

- A determination was started in the Sample list.
- Before the subsample determination, the **Expiry date exceeded** warning message is displayed.

1 Continuing the determination

- Click on **[Continue]** in the warning message to continue the execution of the subsample despite **Expiry date** having been exceeded.

If the **Prevent determination with expired equipment** function is enabled in the operating procedure under **Properties** ▶ **Execute with**, then the determination can be continued only if the user has been assigned the **Start determinations with expired equipment** user right. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

If the determination is executed with expired equipment, then the measuring results may be flawed.

See also

Sensor – Status (chapter 5.12.6.3, page 1007)

Solution – Definition (chapter 5.12.7, page 1012)

5.8 Signature – Brief description

In the **OMNIS Client/Server system**, the operating procedures and methods can only be signed after publishing. To be able to sign a published operating procedure, all the associated methods must first be signed. Further information on the signature in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Operating procedures, methods and subsamples can be signed on up to 2 levels which then protects them against changes. The following rules apply for this:

- An object can be signed by different users several times on each level.
- Level 2 can only be signed after level 1 has been signed.
- Every user can only sign an object once, regardless of the level of the signature.
- If level 2 has been signed, then level 1 can no longer be signed or deleted.
- Once the object has been signed, then no changes can be made to it. To make any change, first of all, the level 2 signatures and then the level 1 signatures need to be deleted.
- Only executed or canceled subsamples can be signed.
- To sign an operating procedure, first of all the methods it contains must be signed at least on the same level.
- When duplicating an operating procedure/method, the signature is deleted and must be issued again as required.
- When exporting and importing, all signatures are also exported or imported respectively.

- If the operating procedure or method is signed, the assigned work systems are also protected against changes. However, the same functional unit can be replaced by another functional unit of the same type in the work system.

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Creating a signature (chapter 5.8.1, page 198)

Deleting a signature (chapter 5.8.3, page 201)

Displaying signatures (chapter 5.8.2, page 200)

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

5.8.1 Creating a signature

In the **OMNIS Client/Server system**, the operating procedures and methods can only be signed after publishing. To be able to sign a published operating procedure, all the associated methods must first be signed. Further information on the signature in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Operating procedures, methods, and subsamples can be signed and are therefore protected from changes. With the 2 levels of signatures, an approval process e.g. for methods and operating procedures can be applied. To create a new signature, proceed as follows:

1 Selecting the object

Selecting the subsample

To sign subsamples simultaneously, multiple subsamples can be selected by holding the **[CTRL]** key or the **[SHIFT]** key pressed down and clicking on the required subsamples *(see "Editing sample list", chapter 5.10.1.2, page 212)*.

- In the **Samples** work area, the **Sample lists** or **Search queries** subsection, open the sample list or search query.

- Right-click the selected subsample and select **[Add signature]** in the context menu.

Selecting an operating procedure / method

- In the **Processes** work area in the **Operating procedures** or **Methods** subsection, select the desired operating procedure / method.
- Right-click the selected operating procedure / method and select **[Add signature]** in the context menu.

The window for authentication is opened.

2 Authenticating a user

Signatures can only be created if the user has the rights to do so.

- Enter **User ID** and **Password**.
- Click **[Continue]**.

The **Add signature** window opens.

3 Adding a signature

- Select **Sign level 1** or **Sign level 2**.
- Select the **reason for the signature** from the selection list.
- Entering a **Signature comment** is optional.
- Click **[Sign]**.

The object is signed and is marked with (level 1) or (level 2).

Operating procedures or methods must be closed to sign them.

Only executed or canceled subsamples can be signed. Several signatures can be added on both levels.

To sign subsamples, operating procedures or methods, the user must change their password after the account has been newly set up or after their password has been reset by the administrator.

Objects signed at level 1 or level 2 are **locked**, i.e. they cannot be edited or deleted. To edit such objects again, the signatures must first be deleted. When duplicating an operating procedure/method, the signature is deleted and must be issued again as required.

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Deleting a signature (chapter 5.8.3, page 201)

Displaying signatures (chapter 5.8.2, page 200)

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Signature – Brief description (chapter 5.8, page 197)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

5.8.2 Displaying signatures

Information on the signatures in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Signatures for subsamples

1 Opening a sample list or search query

- In **Samples** ▶ **Sample lists**, select the required sample list and open it with a double-click.
  or
- In **Samples** ▶ **Search queries**, select the required search query and open it with a double-click.

2 Selecting the subsample

- Select the subsample for which the signatures are to be shown.

3 Displaying signatures

- Open the **Subsample** ▶ **Signatures** subsection.

The signatures for the selected subsample are displayed.

Signatures for operating procedures or methods

1 Selecting an operating procedure or method

- In **Processes** ▶ **Operating procedures** select the required operating procedure for which the signatures are to be shown.
  or
- In **Processes** ▶ **Methods** select the required method for which the signatures are to be shown.

2 Displaying signatures

- Click on to open the **Properties** window.

The signatures for the selected operating procedure or method are displayed.

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Creating a signature (chapter 5.8.1, page 198)

Deleting a signature (chapter 5.8.3, page 201)

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

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User rights – Directory (chapter 4.5.7.4, page 89)

5.8.3 Deleting a signature

Information on the signature in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

When signatures are deleted, all signatures on the selected level are deleted respectively. To delete existing signatures, proceed as follows:

1 Selecting the object

Selecting the subsample

To delete signatures simultaneously, multiple subsamples can be selected by holding the **[CTRL]** key or the **[SHIFT]** key pressed down and clicking on the required subsamples *(see "Editing sample list", chapter 5.10.1.2, page 212)*.

- In the **Samples** work area, the **Sample lists** or **Search queries** subsection, open the sample list or search query.
- Right-click the selected subsample and select **[Delete signatures]** in the context menu.

Selecting an operating procedure / method

- In the **Processes** work area in the **Operating procedures** or **Methods** subsection, select the desired operating procedure / method.
- Right-click the selected operating procedure / method and select **[Delete signatures]** in the context menu.

The window for authentication is opened.

2 Authenticating a user

Signatures can only be deleted if the user has the rights to do so.

- Enter **User ID** and **Password**.
- Click **[Continue]**.

The **Delete signatures** window opens.

3 Deleting the signatures

First of all, the signatures on level 2 need to be deleted and then the signatures on level 1. The signature level is automatically selected appropriately.

- Entering a **Signature comment** is optional.
- Click **[Delete signatures]**.

The signatures have been deleted.

Operating procedures or methods must be closed to delete signatures.

Objects signed at level 1 or level 2 are **locked**, i.e. they cannot be edited or deleted. To edit such objects again, the signatures must first be deleted.

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Creating a signature (chapter 5.8.1, page 198)

Displaying signatures (chapter 5.8.2, page 200)

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Signature – Brief description (chapter 5.8, page 197)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

5.9 Tags – Definition

Information on the tags in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Tags are used like tags for categorizing and searching in overview lists. Operating procedures, methods, server operating procedures, server methods and quantification models type full can be organized according to tags without moving them into a folder. Multiple tags can be defined for each object. You can thus filter for tags in overview lists.

Those tags are retained during export, import or duplication. If tags are assigned to a quantification model that has already been created, and if it is calculated with the OMD, then the tags for the newly calculated quantification models will be retained.

See also

Creating and editing tags (chapter 5.9.1, page 203)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

5.9.1 Creating and editing tags

- *Create and edit tags*
- *Remove tags*

Newly created tags and any retrospective changes to tags are applied immediately and are saved.
If user management is enabled, then the defined tags are saved by each user for the selected objects. They are still available after restarting the OMNIS Software.

Information on the tags in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Creating and editing tags

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses and function licenses are enabled.
  Additional information: *Metrohm Knowledge Base*

1 Selecting object

- Select the corresponding object in the following areas:
  - **Processes** ▶ **Operating procedures**
  - **Processes** ▶ **Methods**
  - **Models** ▶ **Quantification models**

Tags can be created only for **Quantification model type full**.

- In the **OMNIS Client/Server system**:
  - **Processes** ▶ **Server operating procedures**
  - **Processes** ▶ **Server methods**

2 Opening input field

- Double-click to select the desired field in the **Tags** column.

An input field below the selected line opens.

3 Creating tags

- Write a tag into the input field and confirm with the **[Enter]** or **[Tabulator]** key.

The tag is created and is displayed in the input field as well as in the **Tags** column.

Pay attention to the following when creating tags:
- You may use upper and lower case letters; however, this will not be taken into account when filtering.
- The same tag cannot be assigned twice within an object, even if the use of upper and lower case differs.

4 Selecting existing tags

- Double-click in the input field and select an existing tag from the selection list.
  or
- Write an existing tag in the input field and select it from the selection list.
  or
- Click in the input field and press the downwards **[arrow]** key to mark the desired tag and confirm with another click or with **[Enter]**.

You can select existing tags or recently used tags in the selection list.

5 Renaming tags

- Click on a tag or press the **[backspace]** key to rename the selected tag. Confirm with **[Enter]** or **[Tab]** key.

The tag is renamed only in the selected object.

Removing tags

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Selecting object

- Select the corresponding object in the following areas:
  - **Processes** ▶ **Operating procedures**
  - **Processes** ▶ **Methods**
  - **Models** ▶ **Quantification models**

  In the **OMNIS Client/Server system**:
  - **Processes** ▶ **Server operating procedures**
  - **Processes** ▶ **Server methods**

2 Opening input field

- Double-click to select the desired field in the **Tags** column.

An input field below the selected line opens.

3 Removing individual tags

- Remove individual tags by clicking on ✕ in the tag.
- Alternatively, tags can also be removed with the **[Backspace]** key.

See also

Filtering tags (chapter 5.9.2, page 206)

Method – Definition (chapter 5.11.3, page 413)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Sorting the overview list (chapter 5.2.7, page 171)

Tags – Definition (chapter 5.9, page 203)

5.9.2 Filtering tags

If user management is enabled, the defined tags are saved by each user. They are still available after restarting the OMNIS Software.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Selecting overview list

- Select the corresponding overview list in the following areas:
  - **Samples ▶ Sample profiles**
  - **Processes ▶ Operating procedures**
  - **Processes ▶ Methods**
  - **Models ▶ Quantification models**

  In the **OMNIS Client/Server system**:
  - **Samples ▶ Server sample profiles**
  - **Processes ▶ Server operating procedures**
  - **Processes ▶ Server methods**

2 Filtering by names

Names and tags can be combined to limit the search results further.

- Enter the name of the object you are searching for in the **[Name]** input field.

Only objects that contain the entered term in their name are listed.

Filtering by name is possible in the following subsections:

- Sample profiles
- Operating procedures
- Methods
- Server sample profiles
- Server operating procedures
- Server methods
- Quantification models

3 Filtering by tags

- Enter the name of a tag that is assigned to the object you are looking for in the **[Enter tags]** input field.

Only objects that were assigned the entered tag are listed.

Filtering by tags is possible in the following subsections:

- Operating procedures
- Methods
- Server operating procedures
- Server methods
- Quantification models

See also

Creating and editing tags (chapter 5.9.1, page 203)

Method – Definition (chapter 5.11.3, page 413)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Sample profile – Definition (chapter 5.10.5, page 258)

Tags – Definition (chapter 5.9, page 203)

5.10 Samples – Actions

In the **OMNIS Stand-Alone**, the following actions can be executed in the subsections of the **Samples** work area:

- Samples and subsamples are created, processed, signed and managed in **Samples** ▶ **Sample lists**. The recorded subsamples can then be analyzed directly.
- Control charts are created, processed and managed in **Samples** ▶ **Control charts**. If the values of the control chart are outside the defined limits, then optional runs of the operating procedure can be used as an action.
- Filter criteria which are used to search for samples and subsamples in the database are defined in **Samples** ▶ **Search queries**. Subsamples can be signed and samples can be locked.
- Samples with identical sample data are efficiently recorded in **Samples** ▶ **Sample profiles**. It is also possible to define how many subsamples are to be created automatically using which operating procedures.
- System variables are created, processed and managed in **Samples** ▶ **System variables**. The system variables can be used in methods and operating procedures.

In the **OMNIS Client/Server system**, the following actions can be executed in the subsections of the **Samples** work area:

- Samples and subsamples are created, processed, signed and managed in **Samples** ▶ **Sample lists**. The recorded subsamples can then be analyzed directly.

-

  Control charts are created, processed and managed in **Samples ▶ Control charts**. If the values of the control chart are outside the defined limits, then optional runs of the operating procedure can be used as an action.
-

  Filter criteria which are used to search for samples and subsamples in the database are defined in **Samples ▶ Search queries**. Subsamples can be signed and samples can be locked.
-

  Filter criteria which are used to search for samples and subsamples on the OMNIS Server are defined in **Samples ▶ Server search queries**.
-

  Samples with identical sample data are efficiently recorded in **Samples ▶ Sample profiles**. It is also possible to define how many subsamples are to be created automatically using which operating procedures. Sample profiles can be published.
-

  Published sample profiles are downloaded or deleted from the OMNIS Server in **Samples ▶ Server sample profiles**.
-

  System variables are created, processed and managed in **Samples ▶ System variables**. The system variables can be used in methods and operating procedures.

See also

Control chart – Definition (chapter 5.10.15, page 368)

Creating a signature (chapter 5.8.1, page 198)

Creating and deleting sample lists (chapter 5.10.1.1, page 211)

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Creating system variables (chapter 5.10.14.2, page 366)

Deleting a signature (chapter 5.8.3, page 201)

Locking or unlocking samples (chapter 5.10.4.4, page 257)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Sample list – Tab (chapter 5.2.2, page 159)

Sample profile – Definition (chapter 5.10.5, page 258)

Search queries – Definition (chapter 5.10.2, page 243)

System variables – Definition (chapter 5.10.14, page 365)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.1 Sample lists – Subsection

The following functions are available in **Samples** ▶ **Sample lists**:

- **Create sample list** creates a new sample list in which samples and subsamples can be inserted and edited.
- **Duplicate sample list** duplicates the selected sample list under the same name and with a consecutive number. If a name already ends with a number, then this number is incremented by +1.
  The newly created sample list contains duplicates of the samples and subsamples from the original sample list. The subsamples have the **Ready** status and can be analyzed immediately.
- **Remove sample lists from local OMNIS Client** removes the selected sample lists with all the samples they contain from the local system. Corresponding subsamples that are contained in other sample lists will also be removed. The samples and subsamples are retained on the OMNIS Server.
  Note: Only applicable in the **OMNIS Client/Server system**.
- **Archive samples from sample list** archives the selected sample list with all the samples contained including their subsamples. They are deleted from the database.
- The selected sample lists are deleted with **Delete sample lists**. The samples and subsamples it contains are retained in the database.

Overview list

The following information is displayed in the overview list:

Name	Name of the sample list. The name can be modified after opening the sample list.
Saved	Time at which the sample list was last saved.
Data permissions	Existing data permissions assigned to this sample list. **Note**: Applies only if data permissions are enabled and the user has the necessary user rights.

See also

Data permissions – Definition (chapter 4.5.9, page 105)

Editing sample list (chapter 5.10.1.2, page 212)

Sample list – Tab (chapter 5.2.2, page 159)

5.10.1.1 Creating and deleting sample lists

Creating a sample list

1 Creating a new sample list

- In **Samples** ▶ **Sample lists**, click on .

A new tab opens with **New sample list** as its title.

2 Naming a sample list

- Enter the desired name for the new sample list In the **Name** field and confirm with **[Enter]**.

The name entered is displayed on the tab.

3 Saving a sample list

- Enter samples or subsamples in the sample list*(see "Recording samples", chapter 5.10.4.1, page 251)*.
- Click to save the created sample list.

Deleting sample lists

1 Selecting a sample list

- Select the required sample lists in **Samples** ▶ **Sample lists**.

2 Deleting a sample list

- Delete the selected sample lists by clicking on .

The samples and subsamples contained in the sample lists are retained in the database when the sample lists are deleted and are thus also retained in other sample lists.

See also

Editing sample list (chapter 5.10.1.2, page 212)

Recording samples (chapter 5.10.4.1, page 251)

Recording subsamples (chapter 5.10.7.1, page 273)

5.10.1.2 Editing sample list

- *Renaming a sample list*
- *Selecting objects in the sample list*
- *Deselecting objects in the sample list*
- *Deselecting an intermediate area in the sample list*
- *Editing cells in the sample list*
- *Cutting and pasting samples or subsamples*
- *Copying and pasting samples or subsamples*
- *Adding sample data in the sample list*
- *Inserting sample data from a CSV file*
- *Updating the sample list*
- *Restoring focus*

Save all changes in the sample list by clicking on . All unsaved changes are lost.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

Renaming sample list

1 Renaming sample list

- Enter the desired name in the **Name** field under **Samples ▶ Sample list**.
- Confirm the entry by clicking **[Enter]**.

The new name is automatically entered in the tab.

Selecting objects in the sample list

1 Selecting individual objects

- Click on or to select individual samples or subsamples.

or

- Click on the desired cell to select it.
- Click on additional objects with the **[CTRL]** key pressed to add them to the selection.

For cells, only cells with the same name and same type in the same column can be selected together.

2 Selecting multiple objects

- Click on or to select all samples or subsamples of a group.
- If an object is selected, then clicking a different object with the same type while holding the **[SHIFT]** key pressed down causes all of the cells in between them to be added to the selection.
- If multiple objects are selected, then clicking a different object with the same type with the key combination **[CTRL]**+**[SHIFT]** causes all of the cells in between to be added to the selection.

3 Selecting all objects

- If an object is selected, all objects in the list can be selected with the key combination **[CTRL]**+**[A]**.

Deselecting objects in the sample list

Prerequisite:

- At least one object is selected: *Selecting objects in the sample list*

1 Deselecting individual objects

- Deselect by clicking a selected object while holding the **[CTRL]** key.

2 Deselecting multiple objects

- If multiple objects are selected, all cells outside of the 2 objects can be deselected by clicking on one of the selected objects while holding down the **[SHIFT]** key.

Deselecting an intermediate area in the sample list

Prerequisite:

- Multiple objects are selected: *Selecting objects in the sample list*

1 Deselecting multiple objects within the selected area

- Click on an object within the selected area while holding down the **[CTRL]** key.
- Within the selected area, click on a different object with the same type with the key combination **[CTRL]**+**[SHIFT]**.

All cells in between are deselected.

Editing cells in the sample list

1 Editing content

- Double-click a cell within the sample list.

2 Incrementing content

- Select the required cells within a column.
- Right-click on one of the cells to open the context menu and select **Increment**.

The numerical value of the selected cell at the top is taken as base value for incrementing the selected section.

Incrementing only works for cells that contain a number or a text.

3 Filling content

- Select the required cells within a column.
- Right-click on one of the cells to open the context menu and select **Fill**.

The content of the topmost selected cell is inserted into the other cells of the selected area.

Filling works only for cells that contain a number or a text.

Cutting and pasting samples or subsamples

Prerequisite:

- A sample or subsample is selected: *Selecting objects in the sample list*.

1 Cutting sample or subsample

- Open the context menu by right-clicking the highlighted section and select **[Cut]**.
  or
- Cut the selected sample or subsample with the key combination **[CTRL]**+**[X]**.

Multiple samples and subsamples can be cut and inserted simultaneously.

2 Pasting sample or subsample

- Select the sample or subsample underneath which the new subsample is added.
- Open the context menu by right-clicking the highlighted section and select **[Paste]**.
  or
- Insert the cut sample or subsample with the key combination **[CTRL]**+**[V]**.

If no sample is selected, then the sample or subsample is added to the end of the sample list. The display automatically jumps to the inserted sample or subsample.
Deselect a sample or subsample in the sample list: *Deselecting objects in the sample list*

Copying and pasting samples or subsamples

Prerequisite:

- A sample or subsample is selected: *Selecting objects in the sample list*.

1 Copying sample or subsample

- Open the context menu by right-clicking the highlighted section and select **[Copy]**.
  or
- Copy the selected sample or subsample with the key combination **[CTRL]**+**[C]**.

A sample is copied with all subsamples contained and visible in the sample list. Either multiple samples or multiple subsamples can be copied and pasted simultaneously.

2 Pasting sample or subsample

- Select the sample or subsample underneath which the new subsample or subsample is added.
- Open the context menu by right-clicking the highlighted section and select **[Paste]**.
  or
- Insert the copied sample or subsample with the key combination **[CTRL]**+**[V]**.

The samples and subsamples are inserted as follows:

- The subsamples have the status **Ready**.
- The subsamples contain the most recent version of the operating procedure of the originally copied subsample. If a subsample refers to an operating procedure that no longer exists locally, then this subsample is not inserted. Subsamples with withdrawn operating procedures are inserted.
- The results of the subsamples and the values of the sample data and subsample data with usage type **Result** are reset.
- The other sample data and subsample data have the value of the originally copied sample or subsample. If subsample data has been changed since the copied subsample was determined in the operating procedure, then the inserted subsample will have this changed subsample data. Subsample data with values that cannot be applied from the originally copied subsample has the default value.

Adding sample data in the sample list

1 Adding sample data

- Right-click the selected samples to open the context menu and select **Add sample data**.

2 Defining sample data

- In the **Field name short** field, enter the name for the input field that is used as the column header in the sample list.
- In the **Field name long** field, enter the name for the input field that is used as a designation in reports.
  Note: If no name is entered in the **Field name long** field, then the name in the **Field name short** field will be used in the reports.
- In the **Type of input field** field, select the required type (**Text**, **Number** or **Selection list**).

- Select the required mode of use for the input field in the **Use as** field:
  - **Input field**: Field in which data can be entered (for **Text** or **Number** types).
  - **Result**: Field that can be filled with the corresponding commands during the determination run (**CALC** and **REQUEST**) (for **Text** or **Number** type). This field cannot be edited directly.
  - **User-defined selection list**: Selection list with which a list element can be selected from a list the users have defined themselves (for the **Selection list** type).
  - **Product**: Field in which the user can enter a product name (for the **Text** or **Selection list** type).
- For fields of the **Selection list** type that are used as the product, the **Select elements** button is displayed in the **Properties input field** section. Existing products from the database can be added to the list in the input field by clicking on **Select elements**.
  - For categories of the **Identification models** type: Source shows the most recently published version of all identification models.
  - For category of the **Model hierarchies** type: Source shows the most recently published version of all model hierarchies.
- Enable the **Allow free text** check box to give users the option of creating a list entry themselves in the sample list if the predefined entries are not sufficient. This option is visible only if **Selection list** and **User-defined selection list** or **Product** have been selected.
- Depending on the type and use of the input field, additional fields are displayed in the **Properties input field** section that can be filled out as required.
- Disable the **Editable field** check box if the user should not be able to edit the input field for the sample in the sample list.
- Enable the **Allow empty field** check box if a field without the entry of a value is to be permissible.
- Enable the **Force entry** check box if the entry of a value is to be forced for all empty fields before the determination start. This option is visible only if **Allow empty field** has been enabled.

The **Properties input field** section is not available in the following cases:

- If **Text** or **Number** was selected in **Type of input field** and if **Result** was selected in **Use as**.
- If **Date** was selected in **Type of input field** and if **Determination start** was selected in **Use as**.

Sample data can also be defined in Sample profile. Sample data that is recorded directly in the sample list does not however have an influence on the sample data in the sample profile being used. Additional information on the sample profile: *(see "Creating and editing sample profile", chapter 5.10.5.2, page 261)*

3 Deleting or adding additional input fields

- To add additional input fields, right-click in the text field and select **[Add input field]** or click .
- To delete an input field, right-click the name field and select **[Delete input field]**.

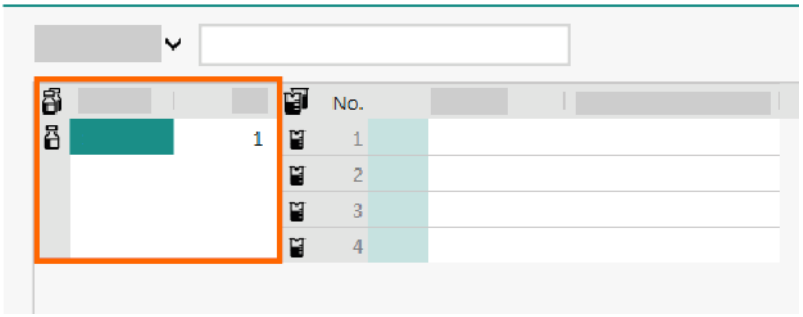
4 Modifying the sequence of sample data (optional)

- Select the required input field by clicking an editable field and move it to the left by clicking or move it to the right by clicking .
  The defined input files are added at the end of the sample data that already exists.

5 Displaying sample data in the sample list

- Click **[Add]** to confirm the changes.

The defined sample data is displayed as column headers for the selected samples in the sample list.



Furthermore, the newly added sample data is also available as variables in the formula editor for subsamples which have not been analyzed.

Inserting sample data from a CSV file

Prerequisite:

- A sample with sample data is available in the sample list.
- A prepared CSV file with sample data is available: *(see "Preparing a CSV file", chapter 5.10.7.6, page 284)*

1 Copying sample data from a CSV file

- Select and copy the lines and columns with the desired sample data, as well as a column with the corresponding sample names together with their headings in the CSV file. The headings of the sample data in the table of the CSV file must be the same as the headings of the sample data in the sample list.

2 Inserting sample data in the sample list

- In the sample list, select the specimens with the sample data that is to be inserted. The selected samples must not be locked or contain subsamples that are being executed.
- Right-click the selected samples to open the context menu.
- Click on **Insert sample data from CSV file** to add the copied sample data from the CSV file to the sample data in the sample list.

When inserting the sample data from a CSV file, the following must be observed:

- Lines and columns of the copied sample data in the CSV file must match the lines and columns of the sample data in the sample list. Furthermore, the table of the CSV file must contain a column with the sample names for the sample assignment.
- No empty cell may be inserted in fields of the sample data where no empty fields are allowed.
- The notation of the decimal separators in the CSV file and the sample data in the sample list must be the same.
- No text may be inserted in fields of type **Number**.

Updating sample list

1 Updating sample list

- Update the sample list including all sample data and subsample data by clicking ↻ or **[F5]**.

Unsaved changes are lost when the sample list is updated.

Restoring focus

1 Restoring focus

- Click on to restore the focus to the currently running subsample and its Live data. The following logic applies to the determination sequence: *(see "Starting determination", chapter 5.10.8.6, page 304)*

See also

Creating and deleting sample lists (chapter 5.10.1.1, page 211)

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Creating report (chapter 5.10.1.4, page 224)

Exporting subsample data (chapter 5.10.1.3, page 220)

Importing subsample data (chapter 5.10.7.7, page 289)

Models – Definition (chapter 5.13.1.1, page 1056)

Recording samples (chapter 5.10.4.1, page 251)

Recording subsamples (chapter 5.10.7.1, page 273)

Run test – Brief description (chapter 5.10.8.1, page 295)

Samples – Actions (chapter 5.10, page 208)

Signature – Brief description (chapter 5.8, page 197)

Subsamples – Statuses (chapter 5.10.7.3, page 276)

5.10.1.3 Exporting subsample data

There are 3 options in the OMNIS Software for exporting subsample data:

- *Automated export* during a determination with the **EXPORT** command: *(see "EXPORT – Parameters", chapter 5.11.8.69, page 780)*
- *Automated export* after a determination has been run.
- *Manual export* from the sample list.

The sample data and subsample data of a determination are exported as **CSV file** (Comma Separated Value). If the file does not exist yet, it is created. If the file already exists, the new determination data is added. The order of the fields for the sample data and subsample data corresponds to the order in the sample list.

The exported file contains at least 2 lines that are separated by CR/LF (Carriage Return / Line Feed). The top line contains the column headings (**Field name short** for sample data and subsample data). The line below contains the field contents.

When exporting subsamples with different column headings in the same file, all column headings are written above the respective data in the file. If subsamples in the file have the same column headings, then they are only written once. All fields are separated from one another with a semicolon (;).

Automated export with the EXPORT command

1 Inserting a command

- Use drag and drop to insert the **EXPORT** command from the Library into the operating procedure or method in **Processes** ▶ **Operating procedures** or **Methods** ▶ .

2 Opening the parameters

- Click on to open the **Properties** window.
  or
- Double-click on the **EXPORT** command to open the **Properties** window directly.

The exports can be defined in **Properties** ▶ **Parameters**.

3 Defining an export

- Select an export type from the selection list in the **Export type** field.
- If the **CSV – Sample data and subsample data** option is selected, then selection can be made in **Export in** as to whether the export is to be executed in **One file** or **Separate files**.
- In the **Target folder** field, select the target folder by clicking or enter the absolute path to which the CSV file is to be saved in the address bar.
- From the selection list **File name**, select an option for the file name under which the export will be saved. The default value **OMNIS_Export** can be changed. The following options are available:
  - Enter the text; the following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9
  - Enter the file name using the formula editor and variable

4 Saving an export

- Save the export settings by clicking .

Automated export from the operating procedure

1 Opening an operating procedure

- In **Processes** ▶ **Operating procedures**, select the required operating procedure and open it with a double-click.

2 Opening Exports

- Click on to open the **Properties** window.
  or
- Double-click on

to open the **Properties** window directly.
- Open the **Properties** ▶ **Exports** subsection.

3 Adding an export

- Click on to add a new export.

4 Defining an export

- Select an export type from the selection list in the **Export type** field.
- If the **CSV – Sample data and subsample data** option is selected, then the export can be executed in **One file** or **Separate files**.
- In the **Target folder** field, select the target folder by clicking on or enter the absolute path in which the export is to be saved in the address bar.
- From the selection list **File name**, select an option for the file name under which the export will be saved. The default value **OMNIS_Export** can be changed. The following options are available:
  - Enter the text; the following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9
  - Enter the file name using the formula editor and variable

5 Saving an export

- Save the export settings by clicking .

Manual export from the sample list

Prerequisite:

- The user has the **Export samples** right.
- The sample list is open.
- The data in the sample list has been saved.

1 Selecting samples and subsamples

- Click on or to select individual samples or subsamples.
  or
- Click on or to select all samples or subsamples of a group.
- To select multiple samples or subsamples, select the required samples or subsamples while pressing down the **[SHIFT]** key or the **[CTRL]** key.

2 Exporting data

- Click on to open the **Export data** window.

3 Defining an export

- Select an export type from the selection list in the **Export type** field.
  - For the **OMNIS – Samples and subsamples** export type, the sample data and subsample data are exported as **Sample data file**.
- Select the option **Selected subsamples** or **All subsamples in the list**.
- If the **CSV – Sample data and subsample data** option is selected, then the export can be executed in **One file** or **Separate files**.
- In the **Target folder** field, select the target folder by clicking on or enter the absolute path in which the export is to be saved in the address bar.
- Enter the name under which the file is to be saved in the **File name** field. The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

4 Creating an OMNIS subsample data file

- Create the OMNIS subsample data file by clicking on **[Export]**.

This may take several minutes.
All time indications for the exported subsamples (e.g. start of determination) are converted into the Coordinated Universal Time (UTC±00:00) when exporting. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.
For the date and time displayed in the file name, the local time on the computer is added in the format **-YYYY-MM-DD-hh-mm-ss-ms** (e.g. **-2017-02-14-08-02-07-549**).

See also

Importing subsample data (chapter 5.10.7.7, page 289)

Recording subsamples (chapter 5.10.7.1, page 273)

Sending data to third-party software (chapter 5.10.7.8, page 291)

5.10.1.4 Creating report

The following options for creating reports are available in the OMNIS Software:

- *Automated report creation* during a determination with the **REPORT** command*(see "REPORT – Parameters", chapter 5.11.8.76, page 793)*.
- *Automated report creation* after running a determination. The setting can be made under **Processes** ▶ **Operating procedures** ▶ **Properties** ▶ **Reports**.
- *Manual report creation* from the sample list.
- *Manual report creation* from the work area **Processes**.
- *Manual report creation* from the work area **Models**.
- *Manual report creation* from the work area **Audit Trail**.
- *Manual report creation* from the work area **User management**.

In the **OMNIS Client/Server system**, the connection to the OMNIS Server is required for creating reports. If the connection to the OMNIS Server was interrupted, it must be re-established in order to create reports.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

Additional prerequisite for manual report creation (optional):

- The **Enable print settings adjustment** check box in **Settings ▶ General settings** is enabled so that the settings **Copies**, **Double-sided printing** and **Color** are available.

Automated report creation with the REPORT command

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Inserting command

- Use drag and drop to insert the **REPORT** command from the Library into the operating procedure or method in **Processes ▶ Operating procedures** or **Methods ▶** .

2 Opening parameters

- Click on to open the **Properties** window.
  or
- Double-click on the **REPORT** command to open the **Properties** window directly.
- Open the **Properties ▶ Parameters** subsection.

3 Defining report

- Select the desired report template from the **Report template** selection list*(see "Report template – Directory", chapter 5.10.1.4.1, page 233)*.
- Select the desired output language from the **Output language** selection list.
- Select the output format **PDF file** or **Paper printout**.
- Select a target folder by clicking in the **Target folder** field. Alternatively, enter the target folder path in which the report is to be saved. If the desired folder does not exist, then it is created when creating the report.

- From the **PDF file name** selection list, select an option for the file name under which the report will be saved. The default value **OMNIS_Report** can be changed. The following options are available:
  - Enter the text; the following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9
  - Enter the file name using the formula editor and variable.

4 Saving report

- Save the report settings by clicking on .

Automated report creation from the operating procedure

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Opening operating procedure

- In **Processes** ▶ **Operating procedures**, select the required operating procedure and open it with a double-click.

2 Opening reports

- Click on to open the **Properties** window.
  or
- Double-click on

to open the **Properties** window directly.
- Open the **Properties** ▶ **Reports** subsection.

3 Adding report

- Click on to add a new report.

4 Defining report

- Select the desired report template from the **Report template** selection list*(see "Report template – Directory", chapter 5.10.1.4.1, page 233)*.
- Select the desired output language from the **Output language** selection list.

- Select the output format **PDF file** or **Paper printout**.
- Select a target folder by clicking in the **Target folder** field. Alternatively, enter the target folder path in which the report is to be saved. If the desired folder does not exist, then it is created when creating the report.
- From the **PDF file name** selection list, select an option for the file name under which the report will be saved. The default value **OMNIS_Report** can be changed. The following options are available:
  - Enter the text; the following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9
  - Enter the file name using the formula editor and variable.

5 Saving report

- Save the report settings by clicking on .

Manual report creation from the sample list

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Selecting samples or subsamples

- Click on or to select individual samples or subsamples.

or

- Click on or to select all samples or subsamples of a group.
- To select multiple samples or subsamples, select the required samples or subsamples while pressing down the **[SHIFT]** key or the **[CTRL]** key.*(see "Editing sample list", chapter 5.10.1.2, page 212)*
- Click on the dialog for the report definition by clicking on .

A report is created for each of the selected samples or subsamples.

Applies for **Sample result report** or **Sample result report (short)**: The sequence in which the subsamples was added to the sample determines the sequence of the subsamples in the report.

Applies to **Subsample result report (Audit Trail)**: All Audit Trail entries that relate to a selected subsample are included in the report. These are the Audit Trail entries that are displayed in the sample list in the **Subsample** ▶ **History** area by clicking on the link **Show Audit Trail**.

2 Defining report

- Select the desired report template from the **Report template** selection list*(see "Report template – Directory", chapter 5.10.1.4.1, page 233)*.
- Select the option **Selected samples** or **Selected subsamples** or select the option **All samples in the list** or **All subsamples in the list**.
- Select the desired output language from the **Output language** selection list.
- Select the **PDF file** output format.
  - For output as PDF file, select the target folder by clicking on . Alternatively, enter the target folder path in which the report is to be saved. If the desired folder does not exist, then it is created when creating the report.
  - Enter the name under which the file is to be saved in the **PDF file name** field. The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

  or
- Select the **Paper printout** output format.
  - Select the required printer from the **Printer** selection list.
  - Enter the required number of copies Input field **Copies**.
  - Enable two-sided printing (optional).
  - Select the required **Color** for printing.

3 Creating report

- Click on **[Create PDF]** to create the report as a PDF file.
  or
- Click on **[Print]** to print the report via the selected printer.

Manual report creation from the Processes work area

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Selecting an operating procedure or method

- Select the corresponding operating procedure or method in the following subsections:
  - **Processes ▶ Operating procedures**
  - **Processes ▶ Method**
- Click on the dialog for the report definition by clicking on .

2 Defining reports

- Select the desired output language from the **Output language** selection list.
- Select the **PDF file** output format.
  - For output as PDF file, select the target folder by clicking on . Alternatively, enter the target folder path in which the report is to be saved.
  - The reports are saved under the name of the respective operating procedure or method. If the name of the operating procedure or method contains one of the special characters > < : " / \ | * ? or CON, PRN, AUX, NUL, COM1 … COM9, LPT1 … LPT9, then these will be replaced by the character **(_)**.

  or
- Select the **Paper printout** output format.
  - Select the required printer from the **Printer** selection list.
  - Enter the required number of copies Input field **Copies**.
  - Enable two-sided printing (optional).
  - Select the required **Color** for printing.

3 Creating reports

- Click on **[Create PDF]** to create a report as a PDF file for each selected operating procedure or method.
  or
- Click on **[Print]** to print a report for each selected operating procedure or method.

Manual report creation from the Models work area

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Selecting model

- Select a corresponding model in the following subsections:
  - **Models ▶ Quantification models**
  - **Models ▶ Slope/y-intercept corrections**
  - **Models ▶ Identification models**
  - **Models ▶ Model hierarchies**
- Click on the dialog for the report definition by clicking on .

2 Defining report

- Select the desired output language from the **Output language** selection list.
- Select the **PDF file** output format.
  - For output as PDF file, select the target folder by clicking on . Alternatively, enter the target folder path in which the report is to be saved.
  - Enter the name under which the file is to be saved in the **PDF file name** field. The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

  or
- Select the **Paper printout** output format.
  - Select the required printer from the **Printer** selection list.
  - Enter the required number of copies Input field **Copies**.
  - Enable two-sided printing (optional).
  - Select the required **Color** for printing.

3 Creating report

- Click on **[Create PDF]** to create the report as a PDF file.
  or
- Click on **[Print]** to print the report via the selected printer.

Manual report creation from the Audit Trail work area

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Opening dialog

- Open the dialog for report definition by clicking on in **Audit Trail**.

2 Defining report

- Select the desired output language from the **Output language** selection list.
- Select the **PDF file** output format.
  - For output as PDF file, select the target folder by clicking on . Alternatively, enter the target folder path in which the report is to be saved.
  - Enter the name under which the file is to be saved in the **PDF file name** field. The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

  or
- Select the **Paper printout** output format.
  - Select the required printer from the **Printer** selection list.
  - Enter the required number of copies Input field **Copies**.
  - Enable two-sided printing (optional).
  - Select the required **Color** for printing.

3 Creating report

- Click on **[Create PDF]** to create the report as a PDF file.
  or
- Click on **[Print]** to print the report via the selected printer.

One report is generated for every 5,000 Audit Trail entries.

Manual report creation from the User management work area

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Opening dialog

- Open the corresponding subsection:
  - **User management ▶ User list**
  - **User management ▶ User roles**
  - **User management ▶ User groups**
- Click on the dialog for the report definition by clicking on .

2 Defining report

- Select the desired output language from the **Output language** selection list.
- Select the **PDF file** output format.
  - For output as PDF file, select the target folder by clicking on . Alternatively, enter the target folder path in which the report is to be saved.
  - Enter the name under which the file is to be saved in the **PDF file name** field. The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

  or
- Select the **Paper printout** output format.
  - Select the required printer from the **Printer** selection list.
  - Enter the required number of copies Input field **Copies**.
  - Optionally enable two-sided printing.
  - Select the required **Color** for printing.

3 Creating report

- Click on **[Create PDF]** to create the report as a PDF file.
  or
- Click on **[Print]** to print the report via the selected printer.

Applying a custom logo

In order to use your own logo, the **logo.png** file in the OMNIS-installation directory under "**...\Metrohm\Desktop\Resources\ReportTemplates**" must be replaced. Local administrator rights are required to be able to make changes in this directory.

The new file must fulfil the following points to be detected by the OMNIS Software:

- File format: BMP, JPG, PNG, TIFF
- File name: **logo.*** (* = bmp, jpg, png, tiff)

- Files with a different file format, but with the same file name, can be saved in the same folder.
- The file size must not exceed 500 kB. The logo is automatically scaled to the maximum height (9 mm) and/or maximum width (470 mm). The proportions (relation height/width) of the logo are maintained.
- The logo is used for all report templates.

See also

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Data permissions – Definition (chapter 4.5.9, page 105)

General settings – Subsection (chapter 5.15.3, page 1203)

REPORT – Parameters (chapter 5.11.8.76, page 793)

Report template – Directory (chapter 5.10.1.4.1, page 233)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.1.4.1 Report template – Directory

The following report templates are available for creating reports using the **REPORT** command, an operating procedure or from the sample list. The **Build version** of the OMNIS Software used for creating the respective report is output in the footer of the reports.

Additional information on creating reports: *(see "Creating report", chapter 5.10.1.4, page 224)*

Name	Content
Calibration report (sensor)	Results of the sensor calibration. Data concerning the following is listed therein: ▪ Sample ▪ Subsample – Determination – Operating procedure – Method – Work systems ▪ Calibration data ▪ Curves and data

Name	Content
Sample result report	Results, including curves and data, of all subsamples of a sample.
Sample result report (short)	Data concerning the following is listed therein: ▪ Sample ▪ Sample statistics ▪ Subsample ▪ Determination ▪ Operating procedure ▪ Method ▪ Work systems ▪ Subsample data ▪ Signatures ▪ Results ▪ Result monitoring ▪ Curves and data ▪ Predictions **Note**: The conditioning curves and conditioning data of the **COND CHECK** command are not displayed in the **Sample result report (short)**.
Sample overview report	Statistical summary of the selected sample. Data concerning the following is listed therein: ▪ Sample ▪ Used Operating procedure
Sample list overview report	Tabular overview of all or selected samples and subsamples from a sample list. Data concerning the following is listed therein: ▪ Sample data ▪ Subsample data ▪ Numbering of the columns ▪ Icons for Sample and Subsample ▪ Sample identifications ▪ Status icons of the Subsample ▪ Used Operating procedure ▪ Determination start ▪ Status icons of the Result monitoring ▪ Icons for signatures of Level 1 and Level 2

Name	Content
Subsample equipment report	Data regarding all of the work systems and accessories used for executing the subsample. Data concerning the following is listed therein: ▪ Subsample ▪ Instrument ▪ Work systems with all Functional units ▪ Sensors ▪ Solutions
Subsample process report	Data regarding the operating procedure carried out and the associated methods of the subsample. Data concerning the following is listed therein: ▪ Sample ▪ Subsample ▪ Operating procedure ▪ Signatures ▪ Subsample data ▪ Monitoring ▪ Methods and commands – Method – Work systems – Signatures ▪ Commands with work systems – Solution conditions and Sensor conditions
Subsample result report Subsample result report (short)	Results, including curves and data, of a selected subsample. Data concerning the following is listed therein: ▪ Sample ▪ Subsample – Determination – Operating procedure – Method – Work systems – Subsample data ▪ Signatures ▪ Results ▪ Result monitoring ▪ Curves and data ▪ Predictions **Note**: The conditioning curve and conditioning data of the **COND CHECK** command are not displayed in the **Subsample result report (short)**.

Name	Content
Subsample result report (simplified)	Results, including curves and data, of a selected subsample. Data concerning the following is listed therein: ▪ Sample and subsample ▪ Determination – Operating procedure ▪ Results and monitoring status ▪ Curves and data **Note**: The conditioning curve and conditioning data of the **COND CHECK** command are not displayed. **Note**: In the **Results and monitoring status** section, when any given sample list is selected under **Samples** ► **Sample lists**, only the information under **Results** ► **Calculations** is output.
Subsample result report (Audit Trail)	Results, including curves and data, of a selected subsample. Data concerning the following is listed therein: ▪ Sample ▪ Subsample ▪ Determination ▪ Subsample data ▪ Results ▪ Result monitoring ▪ Curves and data ▪ Operating procedure, Method, Work systems ▪ Signatures ▪ Audit Trail entries that refer to the selected subsample.

Name	Content
Subsample raw data report	Raw data from the determination of a selected subsample. Data concerning the following is listed therein: ▪ Sample ▪ Subsample – Determination – Operating procedure – Method – Work systems – Subsample data ▪ Curves and data **Note**: The raw data can only be represented with limited accuracy in the report. If you require greater accuracy, you can export the raw data as a CSV file and use it in a subsequent evaluation. Additional information in *(see "EXPORT – Parameters", chapter 5.11.8.69, page 780)* **Note**: For determinations with very large measuring point lists (several thousand measuring points), this report cannot be created, depending on the computing power of the computer used.
Subsample history report	Data regarding the subsample and the determination. Data concerning the following is listed therein: ▪ Subsample ▪ Determination ▪ Signatures ▪ History overview

Reports without template selection

In the work areas **Processes**, **Models**, **Audit Trail** and **User management**, the possibility also exists of creating reports directly. The following report types are available:

Name	Content
Report – Operating procedure	Parameters of a selected operating procedure. Data concerning the following is listed therein: ▪ Operating procedure ▪ Signatures ▪ Subsample data ▪ Result monitoring ▪ Methods and commands

Name	Content
Report – Method	Parameters of a selected method. Data concerning the following is listed therein: ▪ Method ▪ Signatures ▪ Work systems ▪ Method variables ▪ Commands with work systems – Solution conditions and Sensor conditions
Report – quantification model	Parameters and data of a selected quantification model. Data concerning the following is listed therein: ▪ Quantification model type full ▪ Properties ▪ Quantification model type light ▪ Wavelength range ▪ Data preprocessing ▪ Figures of merit ▪ Correlation plot ▪ Spectra list
Report – quantification model (short)	Parameters and data of a selected quantification model (short). Data concerning the following is listed therein: ▪ Last published version ▪ Wavelength range ▪ Data preprocessing ▪ Figures of merit
Report – slope/y-intercept correction	Parameters and data of a selected slope/y-intercept correction.
Report – identification model	Parameters and data of a selected identification model. Data concerning the following is listed therein: ▪ Identification model type full ▪ Properties ▪ Identification model type light ▪ Product list ▪ Wavelength range ▪ Data preprocessing ▪ Validation overview ▪ Validation results

Name	Content
Report – identification model (short)	Parameters and data of a selected identification model (short). Data concerning the following is listed therein: ▪ Last published version ▪ Product list ▪ Wavelength range ▪ Data preprocessing ▪ Validation overview
Report – Model hierarchy	Parameters and data of a selected model hierarchy. Data concerning the following is listed therein: ▪ Model hierarchy type full ▪ Properties ▪ Model hierarchy type light ▪ Model hierarchy structure ▪ Validation overview ▪ Validation results
Report – Audit Trail	Data on Audit Trail entries that correspond to the currently applied filter criteria. Data concerning the following is listed therein: ▪ Object properties of the respective Audit Trail entry ▪ Detail view ▪ Changed values
Report – User list and user groups	Data on existing users and user groups. Data concerning the following is listed therein: ▪ User list – User ID – User name – User status – User groups – User roles – Last login ▪ User groups – Name of user group – Active Directory group – Number of members – Created

Name	Content
Report – User groups and data permissions	Data on the existing user groups, the assigned user roles and data permissions. Data concerning the following is listed therein: ▪ User groups and user roles – Name of user group – User roles – Number of members – Created ▪ User groups and data permissions – Name of user group – Data permissions – Automatic assignment – Created
Report – User roles and user rights	Data on existing user roles and user rights. Data concerning the following is listed therein: ▪ User roles ▪ User rights

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Creating report (chapter 5.10.1.4, page 224)

Data permissions – Definition (chapter 4.5.9, page 105)

EXPORT – Parameters (chapter 5.11.8.69, page 780)

Exporting subsample data (chapter 5.10.1.3, page 220)

General settings – Subsection (chapter 5.15.3, page 1203)

Operating procedure – Properties (chapter 5.11.1.2, page 383)

REPORT – Parameters (chapter 5.11.8.76, page 793)

Result monitoring – Status (chapter 5.10.13.4.1, page 355)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.1.5 Sample list – Overview of functions

Information on the sample list in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Available functions in the program as a whole: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

- *Functions with key combinations*

- *Functions with mouse clicks*
- *Functions with key combinations and mouse clicks*

Functions with key combinations

[F5]	**Update view** Reload the sample list. All entries are reloaded. If there are unsaved changes, then these will be discarded.
[CTRL]+[A]	**Select all data** Select all data.
[CTRL]+[B]	**Adding samples based on the sample profile IDs** Open the **Add samples based on the sample profile IDs** dialog.
[CTRL]+[C]	**Copy** Copy the selected sample or subsample or selected table lines to the clipboard.
[CTRL]+[S]	**Save** Save all changes.
[CTRL]+[V]	**Paste** Paste the sample or subsample from the clipboard at the selected position.
[CTRL]+[X]	**Cut** Cut the selected sample or subsample and copy it to the clipboard.
[DELETE]	**Remove** Remove the selected sample or subsample from the sample list.
[CTRL]+[DELETE]	**Delete** Delete the selected sample or subsample permanently from the database.
[CTRL]+[SHIFT]+[HOME]	**Jump to the first line** Jump to the start of the sample list.
[CTRL]+[SHIFT]+[END]	**Jump to the last line** Jump to the end of the sample list.

[ENTER]	**Adding samples based on the sample profile IDs** Add the samples contained in the entered sample profile to the sample list with the **Add samples based on the sample profile IDs** dialog open.
[PAGE UP]	**Scroll upwards** Scroll upwards in the sample list.
[PAGE DOWN]	**Scroll downwards** Scroll downwards in the sample list.

Functions with mouse clicks

Left mouse click	**Select an object** Select an object.
Right mouse-click	**Open context menu** Open context menu with functions for the selected object.
Double-click	**Mark entire word** Within an input field, mark the selected word.

Functions with key combinations and mouse clicks

[CTRL]+ left mouse click	**Add a single object to the selection** Add another object of the same type to the selection by clicking with the **[CTRL]** key pressed. **Deselect single object** Deselect by clicking a selected object while holding the **[CTRL]** key.
[SHIFT]+ left mouse click	**Add several objects to the selection** If an object is selected, then clicking a different object with the same type while holding the **[SHIFT]** key pressed down causes all of the cells in between them to be added to the selection.
[CTRL]+**[SHIFT]** + left mouse click	**Selecting area** If multiple objects are selected, then clicking a different object with the same type with the key combination **[CTRL]**+**[SHIFT]** causes all of the cells in between to be added to the selection.

See also

Creating and deleting sample lists (chapter 5.10.1.1, page 211)

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Editing sample list (chapter 5.10.1.2, page 212)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Recording samples (chapter 5.10.4.1, page 251)

Recording subsamples (chapter 5.10.7.1, page 273)

Samples – Actions (chapter 5.10, page 208)

5.10.2 Search queries – Definition

A **search query** is a sample list that has been created dynamically. The search query can be configured with filter criteria with which the database is searched for matching entries. The entries found can be saved as a separate sample list in their entirety or transferred to a new sample list individually.

An **Audit Trail search query** is a list of Audit Trail entries that has been created dynamically. The search query can be configured with filter criteria with which the database is searched for matching entries. The entries found can be saved as a separate list in their entirety.

A **search query** can be carried out on the local OMNIS system. With an OMNIS Client/Server system, a **server search query** can furthermore be created to search for samples, subsamples and Audit Trail entries on the OMNIS Server.

See also

Creating Search queries and Server search queries (chapter 5.10.2.2, page 244)

Filtering Search queries and Server search queries (chapter 5.10.2.3, page 246)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Sample list – Tab (chapter 5.2.2, page 159)

Samples – Actions (chapter 5.10, page 208)

Sorting the overview list (chapter 5.2.7, page 171)

5.10.2.1 Search queries – Subsection

The following functions are available in **Samples** ► **Search queries**:

-

  Create search query creates a new search query in which you can search for samples and subsamples using filter criteria. The results can be saved as sample list or search query for later use.

- ✕

  The selected search queries are deleted with **Delete search queries**. The samples and subsamples it contains are retained in the database.

Overview list

The following information is displayed in the overview list:

Name	Name of the search query. The name can be adjusted after opening the search query.
Saved	Time at which the search query was last saved.

See also

Creating Search queries and Server search queries (chapter 5.10.2.2, page 244)

Filtering Search queries and Server search queries (chapter 5.10.2.3, page 246)

Search queries – Definition (chapter 5.10.2, page 243)

Search query – Tab (chapter 5.2.3, page 164)

5.10.2.2 Creating Search queries and Server search queries

Creating a search query or a server search query

1 Setting up a search query or server search query

- In **Samples** ▶ **Search queries**, click on .
  or
- In **Samples** ▶ **Server search queries**, click on .

A new tab with an empty search query or server search query is opened.

A server search query searches for samples and subsamples on the OMNIS Server in an **OMNIS Client/Server system**. Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

2 Naming a search query or server search query

- Enter the desired name in the name field and confirm it with **[Enter]**.

3 Configuring filter criteria

- Open the filter and define the required filter criteria by clicking on .

Further information on filtering search queries and server search queries: *(see "Filtering Search queries and Server search queries", chapter 5.10.2.3, page 246)*

4 Saving a search query or server search query

- Save the search query by clicking on .

The name entered is displayed on the tab.

5 Saving found entries

Select from the following options for saving the results of a local search query:

- Click on and select the **Save as new search query** option to save the configured filter criteria as a new search query.
- Click on and select the **Save as new sample list** option to save the samples and subsamples that have been found with the configured filter criteria as a new sample list.
- Click on to move selected subsamples to a new sample list. The subsamples also remain in the original sample list.

Select from the following options for saving the results of a server search query:

- Click on and select the **Save as new server search query** option to save the configured filter criteria as a new server search query.

See also

Filtering Search queries and Server search queries (chapter 5.10.2.3, page 246)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Sample list – Tab (chapter 5.2.2, page 159)

Search queries – Definition (chapter 5.10.2, page 243)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.2.3 Filtering Search queries and Server search queries

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Opening a search query or server search query

- In **Samples** ▶ **Search queries** or **Server search queries**, select the required search query and open it with a double-click.

2 Opening filter

- Open the filter by clicking on .

The area for selecting configurable filter criteria is opened.

3 Selecting logical connective

Select a logical connective from the selection list:

- **All filter criteria must be met**
  - Only search results matching all the selected filter criteria will be displayed in the list.
- **At least one filter criterion must be met**
  - Search results matching at least one filter criterion will be displayed in the list.

4 Adding filter criterion

- Add a filter criterion by clicking on .

Any number of filter criteria can be added to refine the search.

5 Selecting filter criterion

- Select a filter criterion from the selection list.

Depending on the filter criterion, a variety of search operators and options to choose from are available.

6 Defining filter criterion further

- Select a search operator from the selection list, if necessary:
  - **Contains**
    Finds the entries that contain the input in the defined filter criterion.
  - **Equals**
    Finds the entries for which the value in the defined filter criterion corresponds exactly with the input.
  - **Does not equal**
    Finds the entries for which the value in the defined filter criterion does not correspond with the input.
- Then enter or select a search term, a number of days, a value or a date, depending on the filter criterion selected previously.
  If no selection list with search operators is displayed, the required value for the filter criterion can be entered directly.

7 Further defining sample data and subsample data (optional)

If the **Sample data** or **Subsample data** filter criterion is selected, additional fields will open:

- **Field name short**
  Exact designation of self-defined sample data and subsample data used as column header in the sample list. As soon as something is entered in the field, suggestions for completion are displayed.

- **Selection list with the search operators:**
  For test or selection list:
  - **Contains**
    Finds the entries that contain the input in the defined filter criterion.
  - **Equals**
    Finds the entries for which the value in the defined filter criterion corresponds exactly with the input.
  - **Does not equal**
    Finds the entries for which the value in the defined filter criterion does not correspond with the input.

  For number:
  - **Is**
    Finds the entries for which the value in the defined filter criterion corresponds exactly with the input.
  - **Is less than**
    Finds the entries for which the value in the defined filter criterion is smaller than the input.
  - **Is less than or equal to**
    Finds the entries for which the value in the defined filter criterion is smaller than the input or the same as the input.
  - **Is greater than**
    Finds the entries for which the value in the defined filter criterion is larger than the input.
  - **Is greater than or equal to**
    Finds the entries for which the value in the defined filter criterion is larger than the input or the same as the input.

Only the search operators of the corresponding field type are displayed for the selected sample data or subsample data.

- Then enter a search term or a value, depending on the filter criterion selected previously.
  If no selection list with search operators is displayed, the required value for the filter criterion can be entered directly.

8 Filtering

- Apply the selected filter criteria by clicking on **[Filter]**.

The results are displayed in the list according to the filter criteria.

9 Selecting page

- Click on ← or → to display the next or the previous page of the list.
- Click on ⇤ or ⇥ to display the first or the last page of the list.

- Alternatively, enter the page number directly in the input field and confirm with **[Enter]**.

The selected page is displayed.

If samples or subsamples in a sample list have been changed in the meantime, click on to update the list.
The filter is reapplied when the pages are changed.

10 Resetting filter

- Reset changes to the filter criteria to the last status saved by clicking on **[Reset]**.

The results are displayed in the list according to the filter criteria.

11 Deleting a filter criterion

- Delete the filter criterion by clicking on .

If a filter criterion is deleted, then the filter needs to be applied again to see the corresponding entries.

12 Closing filter

- Click on or to close the filter.

The filter criteria remain active, even after closing the filter.

The area for selecting configurable filter criteria is closed.

13 Saving a search query or server search query

- Changes are saved by clicking on .

Further options for saving configured filter criteria can be displayed by clicking on .
Additional information on creating search queries: *(see "Creating Search queries and Server search queries", chapter 5.10.2.2, page 244)*.

Specific filter criteria

- Use the **Monitoring status** filter criterion to find the results of the result monitoring under **Samples** ▶ **Sample list** ▶ **Results** ▶ **Monitoring**. Additional information: *(see "Filtering the monitoring status", chapter 5.10.13.4.2, page 357)*

- With the **Subsample created by**, **Subsample saved by** or **Determination started by** filter criterion, the user who performed the action can be searched for (by user ID) under **Samples** ▶ **Sample lists** ▶ **Subsample** ▶ **History**. Additional information: *(see "Sample list – Tab", chapter 5.2.2, page 159)*
- With the **Calculation result** filter criterion, invalid results from the **Result value** column can be found under **Samples** ▶ **Sample lists** ▶ **Results** ▶ **Calculations**. Additional information: *(see "Calculations – Definition", chapter 5.10.13.1, page 348)*
- With the **Predicted results** filter criterion, the results of the prediction can be found under **Samples** ▶ **Sample lists** ▶ **Results** ▶ **Predictions**. Additional information: *(see "Sample list – Tab", chapter 5.2.2, page 159)*

See also

Calculations – Definition (chapter 5.10.13.1, page 348)

Creating Search queries and Server search queries (chapter 5.10.2.2, page 244)

Filtering the monitoring status (chapter 5.10.13.4.2, page 357)

Sample list – Tab (chapter 5.2.2, page 159)

Search queries – Definition (chapter 5.10.2, page 243)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.3 Server search queries – Subsection

In the **OMNIS Client/Server system**, the following functions are available under **Samples** ▶ **Server search queries**:

-

  Create server search query creates a new search query in which you can search for samples and subsamples on the OMNIS Server using filter criteria. The results can be transferred to a new sample list or saved as a server search query for later use.
-

  The selected server search queries are deleted with **Delete sever search queries**. The samples and subsamples it contains are retained on the OMNIS Server. Search queries that are open cannot be deleted.

Overview list

The following information is displayed in the overview list:

Name	Name of the server search query. The name can be adjusted after opening the server search query.
Saved	Time at which the server search query was last saved.

See also

Creating Search queries and Server search queries (chapter 5.10.2.2, page 244)

Filtering Search queries and Server search queries (chapter 5.10.2.3, page 246)

Search queries – Definition (chapter 5.10.2, page 243)

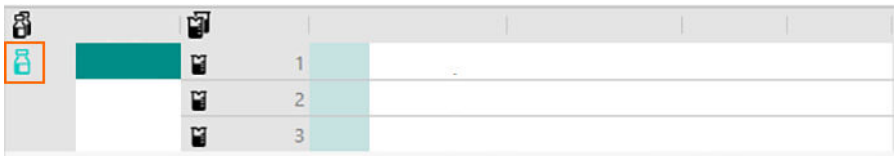
Search query – Tab (chapter 5.2.3, page 164)

5.10.4 Samples – Definition

A sample is the substance to be analyzed. Subsamples which are to be analyzed with the help of an operating procedure are obtained from the sample.

Samples can be identified by various sample data, e.g. name, goods receipt date, batch number, etc. The sample identifications that are to be available as data fields can be specified in a sample profile. This means that various sample profiles can be defined for different kinds of samples.

Example: Sample in the sample list



See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Recording samples (chapter 5.10.4.1, page 251)

5.10.4.1 Recording samples

Information on samples in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

A sample can be added automatically to the sample list during a determination using the **ADD TO SAMPLE LIST** command. Additional information: *(see "ADD TO SAMPLE LIST – Properties", chapter 5.11.8.63, page 761)*

- *Record samples*
- *Record samples based on the sample profile IDs*

Recording samples

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- A sample profile has been created: *(see "Creating and editing sample profile", chapter 5.10.5.2, page 261)*
- A sample list is opened and at the front.

1 Selecting a sample profile

- In the selection list to the left next to the icon, select the suitable sample profile that is to be assigned to the sample.

2 Selecting sample (optional)

- Click on to select the sample under which the new sample is to be inserted.

If no sample is selected, then the sample is automatically added to the end of the sample list. The display automatically jumps to the newly added sample.
Information on deselecting samples: *(see "Editing sample list", chapter 5.10.1.2, page 212)*

3 Adding a sample

- Add a new sample to the sample list by clicking +. The subsamples are added to the sample list automatically in accordance with the sample profile.

4 Naming or renaming sample

- In the **Sample name** column, double-click in the field and enter the name.
- Confirm the entry with the **[ENTER]** button.

The following characters are not allowed: **. | ' " { }**

Creating samples based on the sample profile IDs

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

- A sample profile has been created: *(see "Creating and editing sample profile", chapter 5.10.5.2, page 261)*
- A sample profile ID was assigned to the sample profile: *(see "Creating and editing sample profile", chapter 5.10.5.2, page 261)*
- A sample list is opened and at the front.

1 Selecting sample (optional)

- Click on to select the sample under which the new sample is to be inserted.

If no sample is selected, then the sample is automatically added to the end of the sample list. The display automatically jumps to the newly added sample.
Information on deselecting samples: *(see "Editing sample list", chapter 5.10.1.2, page 212)*

2 Entering a sample profile ID

- Use the key combination **[CTRL]+[B]** or click on to open the **Add samples based on the sample profile IDs** dialog.
- Enter a unique Sample profile ID in the **Sample profile ID** field.

3 Adding a sample

- Click on **[Add]** or **[ENTER]** to add the samples contained in the entered sample profile to the sample list. The subsamples are added to the sample list automatically in accordance with the sample profile.
  The added sample profile IDs are displayed in the **Add samples based on the sample profile IDs** dialog.

Only existing and unique **sample profile IDs** can be added. If the filtering of the data permissions is enabled, then only sample profiles with the data permissions of the currently logged-in user can be added.
Additional information on the data permissions: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

4 Naming or renaming sample

- In the **Sample name** column, double-click in the field and enter the name.
- Confirm the entry with the **[ENTER]** button.

The following characters are not allowed: **. | ' " { }**

See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Editing sample list (chapter 5.10.1.2, page 212)

Recording subsamples (chapter 5.10.7.1, page 273)

Sample list – Overview of functions (chapter 5.10.1.5, page 240)

Sample list – Tab (chapter 5.2.2, page 159)

5.10.4.2 Deleting samples

Information on samples in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

- *Remove samples from the sample list*
- *Delete samples in the sample list*

Removing samples from the sample list

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- A sample list is opened and at the front.
- A sample is selected.

1 Removing sample

- The following options are available for removing a sample:
  - Click – to remove the selected sample from the list. Subsamples that have already been recorded will also be removed at this time.
  - Right-click on the selected sample to open the context menu and select **[Remove from sample list]**.
  - Click the **[DELETE]** key to remove the selected sample.

Removed samples and subsamples are removed only from the current sample list, but still continue to be present in the database.

To find removed samples, a search query can be created in the **Samples** work area.

Deleting samples in the sample list

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- A sample list is opened and at the front.
- A sample is selected.

1 Deleting sample

- The following options are available for deleting a sample:
  - Right-click on the selected sample to open the context menu and select **[Delete]**.
  - Delete the selected sample with the key combination **[CTRL]**+**[DELETE]**.

When deleting a sample, all of the associated subsamples are also permanently deleted in all the sample lists and in the database. This also applies to split samples for which the subsamples are in another location in the same sample list or on other sample lists.

Deleted samples and subsamples are deleted permanently from the database and cannot be restored.

See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Editing sample list (chapter 5.10.1.2, page 212)

Recording subsamples (chapter 5.10.7.1, page 273)

Sample list – Overview of functions (chapter 5.10.1.5, page 240)

Sample list – Tab (chapter 5.2.2, page 159)

5.10.4.3 Archiving samples

Archiving can be planned as a task in **Settings** ▶ **Scheduler**. This automatically archives samples at a defined interval.

The execution of multiple tasks at the same time and for the same samples is not supported. Metrohm recommends defining each task in such a way that it takes other samples into account.

If a task is deleted during its execution, the task is continued until it fails or is terminated. After deleting a task, wait until the scheduled execution time has elapsed before creating a new task for the same samples.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses or function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Archiving sample list

- Select the sample list for which the samples and subsamples are to be archived under **Samples** ▶ **Sample lists**.
- Start archiving by clicking on and continue the process by clicking on **[Archive]**.

A dialog is opened.

Sample lists that are open and have not been saved cannot be archived.

2 Selecting or entering target folder

- Select the target folder or enter the absolute path in the address bar that the archived OSIN files are to be saved in.

If a new folder is created, the following special characters or character strings may not be used: > < : " / \ | * ? and CON, PRN, AUX, NUL, COM1 … COM9, LPT1 … LPT9

3 Creating archive file

- Click on **[Select folder]**.

A dialog is opened. This dialog shows the number of samples to be archived and the number of samples already archived.

The samples in the selected sample list are archived along with their subsamples and an Audit Trail entry is created. The OSIN files are exported to and saved in the target folder. The samples are deleted from the database. The sample list will also be deleted.

This may take several minutes.
Subsamples of a sample that is to be archived that are located in another sample list are also archived and subsequently will no longer be displayed in that other sample list.

Archiving can be stopped by clicking on **[Cancel]**. Samples that have already been archived remain archived and have been deleted from the database.

All time indications are converted into Coordinated Universal Time (UTC±00:00) when archiving. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.
The local time on the computer is used for the date and time displayed in the file name.

See also

Archiving Audit Trail (chapter 5.14.9, page 1192)

Audit Trail – Actions (chapter 5.14, page 1171)

Exporting operating procedures and methods (chapter 5.11.1.5, page 393)

Exporting subsample data (chapter 5.10.1.3, page 220)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.4.4 Locking or unlocking samples

Samples can only be locked or unlocked if the user has the rights to do so.

Samples can be locked which then protects them against the data being changed. If a sample is locked, then no further sample data can be edited and no subsamples can be added or deleted. However, the subsample data can still be changed.

Locking samples

1 Opening a sample list or search query

- In **Samples** ▶ **Sample lists**, select the desired sample list and open it with a double-click.
  or
- In **Samples** ▶ **Search queries** select the desired search query and open it with a double-click.

2 Locking samples

To lock a sample, no changes to be saved may be made. Otherwise the samples list must be saved first.
Samples can be multi-selected *(see "Editing sample list", chapter 5.10.1.2, page 212)*.

- Right click the selected samples and select **[Lock]** in the context menu.

The samples are locked and are marked with .

Unlocking samples

1 Opening a sample list or search query

- In **Samples** ▶ **Sample lists**, select the desired sample list and open it with a double-click.
  or
- In **Samples** ▶ **Search queries** select the desired search query and open it with a double-click.

2 Unlocking samples

Samples can be multi-selected *(see "Editing sample list", chapter 5.10.1.2, page 212)*.

- Right-click the selected samples and select **[Unlock]** in the context menu.

The samples are unlocked.

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Editing sample list (chapter 5.10.1.2, page 212)

General settings – Subsection (chapter 5.15.3, page 1203)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.5 Sample profile – Definition

Information on the sample profile in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

A sample profile is a template for creating samples. This template is used to define which sample data is available for sample identification. In addition, the number of subsamples per sample to be created automatically as well as which operating procedure is to be used to analyze these subsamples can be defined.

Sample profiles are created in **Samples** ▶ **Sample profiles**.

If a sample profile is used to record new samples, the column headers and input fields with standard data are automatically inserted in the sample list. The sample data and subsample data can then be edited individually.

The sample data is also available as '*Name*.**CurrentSampleData**' variables in the formula editor.

See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

5.10.5.1 Sample profiles – Subsection

Information on the sample profile in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The following functions are available in **Samples** ▶ **Sample profiles**:

-
  A new sample profile is created with **Create sample profile** to facilitate the entry of recurrent sample data.
-
  Import sample profile imports one or more OSPR files (**O**MNIS **S**ample **Pr**ofile) as sample profiles. If the sample profiles contain operating procedures, then these will also be imported.
-
  Export sample profiles exports all selected sample profiles as OSPR files (**O**MNIS **S**ample **Pr**ofile). If the sample profiles contain operation procedures, then these will also be exported.
-
  Duplicate sample profiles duplicates the selected sample profiles under the same name and with a consecutive number. If a name already ends with a number, this number is interpreted as the index and it is incremented by +1.
  The newly created sample profiles contain the same sample data and operating procedures as the original sample profiles.
-
  Delete sample profiles deletes all selected sample profiles. Samples that have previously been entered with these sample profiles are retained in the database.
  Note: Only applicable in **OMNIS Stand-Alone**.

-

  Delete server sample profiles removes all selected sample profiles from the local system. If an unpublished sample profile was selected, it is permanently deleted. If the selected sample profiles are being published, then they will be retained on the OMNIS Server. Samples that have previously been entered with the sample profiles are retained in the database in both cases.
  Note: Applicable only in the **OMNIS Client/Server system**.

The sample profiles can be filtered by name. Additional information on filtering sample profiles: *(see "Filtering tags", chapter 5.9.2, page 206)*

Overview list

The following information is displayed in the overview list:

Name	Name of the sample profile. The name can be modified after opening the sample profile.
Published	Status of the sample profile in the **OMNIS Client/Server system**. Additional information: *(see "Sample profiles – Status", chapter 5.10.5.6, page 269)* **Note**: Applicable only in the **OMNIS Client/Server system**.
Saved	Time at which the sample profile was last saved.
Version	Version number of the sample profile. A new version is created automatically each time the sample profile is saved.
Data permissions	Existing data permissions assigned to this sample profile. **Note**: Applies only if data permissions are enabled and the user has the necessary user rights.

See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Data permissions – Definition (chapter 4.5.9, page 105)

Exporting sample profiles (chapter 5.10.5.4, page 266)

Importing sample profiles (chapter 5.10.5.3, page 265)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Sample profile – Definition (chapter 5.10.5, page 258)

Sample profile – Tab (chapter 5.2.4, page 166)

5.10.5.2 Creating and editing sample profile

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Setting up the sample profile

- In **Samples** ▶ **Sample profiles**, click on .

A new tab opens with **New sample profile** as its title.

To edit an existing sample profile, select the required sample profile from the list in **Samples** ▶ **Sample profiles** and open it by double-clicking on the name.
Changes to the sample profile do not affect samples that have already been entered using the sample profile.

2 Naming or renaming sample profile

- Enter the desired name in the **Name of the sample profile** field.

After confirmation with **[ENTER]**, the new name is entered on the tab automatically.

3 Entering sample profile ID (optional)

- Enter a unique designation in the **Sample profile ID** field.

The following special characters must not be used: . | ' " { }

4 Adding sample data

- To add additional sample data, right-click in the text field and select **[Add input field]** or click on .

A new input field is added on the right.

To delete sample data, right-click in the text field and select **[Delete input field]**.

Sample data can also be added directly in the sample list. The sample data that is recorded directly in the sample list does not however have an influence on the sample data in the sample profile being used. Additional information on the adding of sample data in the sample list: *(see "Editing sample list", chapter 5.10.1.2, page 212)*

5 Defining sample data

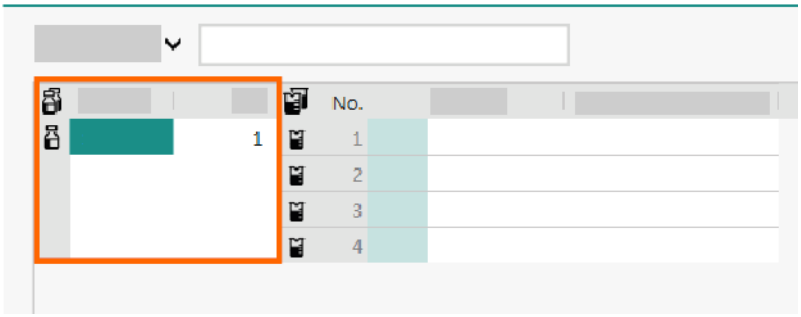
- Enter the name for the input field that is to be used as column header in the sample list in the **Field name short** field for each new entry.
- Enter the name for the input field that is to be used as designation in reports in the **Field name long** field for each new entry. **Note:** If no name is entered in the **Field name long** field, then the name in the **Field name short** field will be used in the reports.
- Select the required type (**Text**, **Number** or **Selection list**) for the information in the **Type of input field** field.
- Select the required mode of use for the input field in the **Use as** field:
  - **Input field**: Field in which the user can enter data (for the **Text** or **Number** type).
  - **Result**: Field that can be filled with the corresponding commands during the determination run (**CALC** and **REQUEST**) (for when type = **Text** or **Number**). This field cannot be edited directly by the user.
  - **User-defined selection list**: Selection list with which users can select a list element from a list they have defined themselves (for type = **Selection list**).
  - **Product**: Field in which the user can enter a product name (for the **Text** or **Selection list** type).
- Depending on the type and use of the input field, additional fields are displayed in the **Properties input field** section that can be filled out as required:
  - For fields of the **Text** type that are used as input fields: **Default value**
  - For fields of the **Number** type that are used as input fields: **Default value**, **Minimum value**, **Maximum value**, **Unit**
  - For fields of the **Selection list** type: **List elements**, **Default value**

- For fields of the **Selection list** type that are used as the product, the **Select elements** button is displayed in the **Properties input field** section. Existing products from the database can be added to the list in the input field by clicking on **Select elements**.
  - For categories of the **Identification models** type: Source shows the most recently published version of all identification models.
  - For category of the **Model hierarchies** type: Source shows the most recently published version of all model hierarchies.
- Enable the **Allow free text** check box to give users the option of creating a list entry themselves in the sample list if the predefined entries are not sufficient. This option is visible only if **Selection list** and **User-defined selection list** or **Product** have been selected.
- Disable the **Editable field** check box if the user should not be able to edit the input field for the sample in the sample list.
- Enable the **Allow empty field** check box if a field without the entry of a value is to be permissible.
- Enable the **Force entry** check box if the entry of a value is to be forced for empty fields before the determination is started. This option is visible only if **Allow empty field** has been enabled.

The **Properties input field** section is not available in the following cases:

- If **Text** or **Number** was selected in **Type of input field** and if **Result** was selected in **Use as**.
- If **Date** was selected in **Type of input field** and if **Determination start** was selected in **Use as**.

The names of the sample data defined in the sample profile are displayed as column headers in the sample list as soon as samples are recorded with this sample profile.



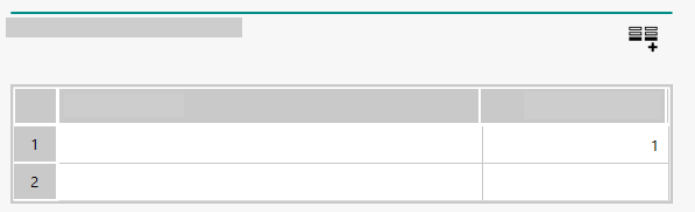
To delete an input field, right-click the name field and select **[Delete input field]**.

6 Modifying the sequence of sample data (optional)

- Select the required input field by clicking an editable field and move it to the left by clicking or move it to the right by clicking .

7 Defining the operating procedure and the number of subsamples

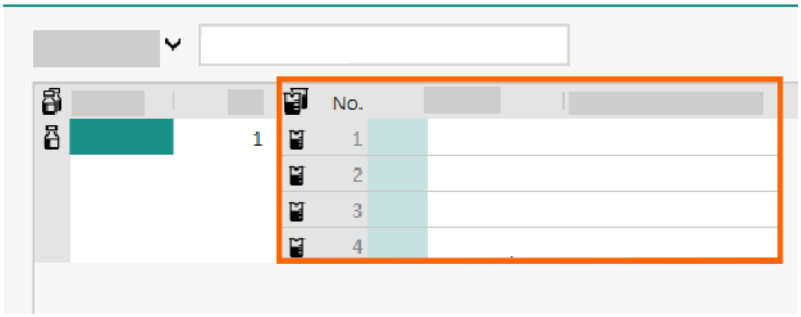
- In the **Operating procedures / subsamples** area, define the operating procedures and the associated number of subsamples that are added automatically to the sample list along with the sample data.
  To add a new line, right-click in the table and select **[Add new row]** or click on .



Several subsamples with operating procedures can be defined per sample profile. The table can also be left empty; operating procedures are optional in the sample profile.

All operating procedures defined in the sample profile are displayed regardless of the data permissions of the logged-in user. If the current user lacks data permissions, then the operating procedures concerned will appear grayed out and cannot be changed by that user. The user can also remove grayed-out operating procedures from the sample profile. This step cannot be undone after saving.

The operating procedures and the associated number of subsamples are automatically added to the sample list as soon as samples are recorded with the created sample profile.



To delete a line, right-click on the selected table row and select **[Delete row]**.

8 Saving a sample profile

- Save the sample profile by clicking on .

In the **OMNIS Client/Server system**, a sample profile can be published after saving it. Information on publishing sample profiles: *(see "Publishing the sample profile", chapter 5.10.5.5, page 267)*

See also

Publishing the sample profile (chapter 5.10.5.5, page 267)

Recording samples (chapter 5.10.4.1, page 251)

Sample profile – Definition (chapter 5.10.5, page 258)

Sample profiles – Status (chapter 5.10.5.6, page 269)

Sample profiles – Subsection (chapter 5.10.5.1, page 259)

Server sample profile – Definition (chapter 5.10.6, page 270)

Variables – Directory (chapter 5.11.9.3, page 827)

5.10.5.3 Importing sample profiles

Prerequisite:

- At least one OSPR file is available.
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting sample profiles

- Click on to open the **Importing sample profiles** window in **Samples** ▶ **Sample profiles**.

2 Browsing for folder

- Select the folder in which the desired sample profiles are saved.

3 Selecting the file

- Select the OMNIS sample profile files or enter the names of the OMNIS sample profile files in the **File name** field.

4 Confirming and importing the selection

- Click **[Open]** to confirm the selection.

The sample profiles have been imported into the OMNIS Software.

If the sample profiles contain operating procedures, then these will also be imported.

See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Exporting sample profiles (chapter 5.10.5.4, page 266)

Importing the templates (chapter 3.2, page 11)

Sample profile – Definition (chapter 5.10.5, page 258)

Sample profiles – Subsection (chapter 5.10.5.1, page 259)

5.10.5.4 Exporting sample profiles

Prerequisite:

- At least one sample profile is available in the overview list.
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting sample profiles

- Select the required sample profiles under **Samples** ▶ **Sample profiles** and open the **Exporting sample profiles** window by clicking on .

2 Selecting an export option

- Enable the **Selected sample profiles** check box to export all of the sample profiles highlighted in the overview list.
- Enable the **All sample profiles** check box to export all sample profiles from the overview list.

3 Selecting or entering a target folder

- Select the target folder or enter the absolute path in the address bar that the sample profiles are to be saved in as an OSPR file.

4 Confirming and exporting the selection

- Click on **[Export]** to confirm the selection.

Depending on the selection, one or more OSPR files are exported under the respective names of the sample profiles. Click on **[Open target folder]** to open the target folder. If the sample profiles contain operating procedures, then the operating procedures will also be exported.

The files are saved under the name of the respective sample profiles. If the name of a sample profile contains one of the special characters > < : " / \ | * ? or CON, PRN, AUX, NUL, COM1 … COM9, LPT1 … LPT9, then these will be replaced by the character **(_)**.

All time indications are converted into Coordinated Universal Time (UTC±00:00) when exporting. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.

The local time on the computer is used for the date and time displayed in the file name.

See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Importing sample profiles (chapter 5.10.5.3, page 265)

Sample profile – Definition (chapter 5.10.5, page 258)

Sample profiles – Subsection (chapter 5.10.5.1, page 259)

5.10.5.5 Publishing the sample profile

Sample profiles can be published in the **OMNIS Client/Server system**.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The **OMNIS Client/Server system** is set up.
- The connection to the OMNIS Server is available.

- All operating procedures in the sample profile are published.

1 Selecting a sample profile

- Create a new sample profile. *(see "Creating and editing sample profile", chapter 5.10.5.2, page 261)*
  or
- In **Samples** ▶ **Sample profiles**, select an existing sample profile and open it with a double-click.

A tab with the newly created or the selected sample profile opens.

2 Calling up the dialog

- Open the **Publish sample profile** dialog by clicking on .
- In the **Name suffix** field, enter the required name suffix for the sample profile that is to be published.

The following special characters must not be used: . | ' " { }
The name suffix is added only to the selected sample profile.
The field for the name of the sample profile is pre-filled and cannot be edited.

3 Publishing the sample profile

- Publish the sample profile by clicking on **[Publish]**.

The published sample profile is marked under **Samples** ▶ **Server sample profiles** with . Under **Samples** ▶ **Sample profiles**, it is marked with only in the overview list of the OMNIS Client that published the sample profile.

If the sample profile contains data permission and this is to be displayed to another user group with different data permissions, then the sample profile must be published once again.

Available data permissions for a sample profile that has already been published can be changed in the overview list under **Samples** ▶ **Sample profiles**. The data permissions are updated for the corresponding server sample profile and this does not create a new server sample profile. Additional information on data permissions: *(see "Assigning data permissions", chapter 4.5.9.2, page 112)*

Published sample profiles are available to all connected OMNIS Clients in the overview list under **Samples** ▶ **Server sample profiles**. They must first be downloaded in order to be subsequently used for a determination. Downloaded sample profiles can be adapted and saved with the changes on the local OMNIS Client. To save the changes of a downloaded sample profile on the OMNIS Server, the sample profile must be republished. Further information on the server sample profiles: *(see "Server sample profile – Definition", chapter 5.10.6, page 270)*

A published sample profile is a copy of the unpublished sample profile. The unpublished sample profile is retained under **Samples** ▶ **Sample profiles** without changes.

When publishing, the name change of the sample profile and the addition or removal of sample data is taken into account. The changed sample profile is published.

To prevent the use of a published sample profile, it can be deleted under **Samples** ▶ **Server sample profiles**. The deleted sample profile is retained locally on connected OMNIS Clients that downloaded the server sample profile before it was deleted. Further information on deleting server sample profiles: *(see "Server sample profiles – Subsection", chapter 5.10.6.1, page 271)*

See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Sample profile – Definition (chapter 5.10.5, page 258)

Sample profiles – Status (chapter 5.10.5.6, page 269)

Sample profiles – Subsection (chapter 5.10.5.1, page 259)

Server sample profile – Definition (chapter 5.10.6, page 270)

Server sample profiles – Subsection (chapter 5.10.6.1, page 271)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.5.6 Sample profiles – Status

In the **OMNIS Client/Server system**, each sample profile that is on the OMNIS Server has a status. This is displayed under **Samples** ▶ **Sample profiles** or **Server sample profiles** in the **Published** column.

Published	Meaning
	Published The sample profile is published. **NOTICE**: Under **Samples** ▶ **Sample profiles**, this status is displayed only in the overview list of the OMNIS Client that published the sample profile.
	Contains withdrawn or deleted objects The sample profile contains at least one withdrawn or deleted operating procedure or method.

The necessary rights must be enabled before a sample profile can be used in a determination. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

See also

Determination – Definition (chapter 5.10.8, page 295)

Determination – Preparation and follow-up (chapter 5.10.8.10, page 313)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Preparing determination (chapter 5.10.8.9, page 310)

Publishing the sample profile (chapter 5.10.5.5, page 267)

Sample profile – Definition (chapter 5.10.5, page 258)

Server sample profile – Definition (chapter 5.10.6, page 270)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.6 Server sample profile – Definition

A **Server sample profile** is understood to be a sample profile that is located on the OMNIS Server and is thus available to all connected OMNIS Clients.

A server sample profile is a template for creating samples. This template is used to define which sample data is available for sample identification, how many subsamples per sample are to be created automatically and with which operating procedures these subsamples are to be analyzed.

Prerequisite for the use of a server sample profile:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The server sample profile has already been downloaded and is available under **Samples** ▶ **Sample profiles**. The associated server operating procedures, server methods and work systems are also downloaded when a server sample profile is downloaded.

A server sample profile can be downloaded in **Samples** ▶ **Server sample profiles** by clicking on .

- The associated methods have at least one **work system** assigned.

After downloading, all functional units of the published work system must be replaced by functional units from custom devices via drag-and-drop and the work system must be saved. No additional functional units can be added to a published work system, nor can any functional units be removed from it.

See also

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Server sample profiles – Subsection (chapter 5.10.6.1, page 271)

5.10.6.1 Server sample profiles – Subsection

The following functions are available in **Samples** ▶ **Server sample profiles**:

-
  Download sample profiles downloads all selected sample profiles and the associated sample data (operating procedures, methods, work systems). The downloaded sample profiles are displayed under **Samples** ▶ **Sample profiles** and can be used.
-
  Update view updates the list of the server sample profiles. All entries are reloaded.
-
  Delete server sample profiles deletes all selected server sample profiles. The associated sample data is not deleted when a server sample profile is deleted. The deleted sample profiles are retained locally on the OMNIS Clients which downloaded the server sample profiles before they were deleted.

Server sample profiles can be filtered by name. Additional information on filtering sample profiles: *(see "Filtering tags", chapter 5.9.2, page 206)*

Overview list

The following information is displayed in the overview list:

Name	Name of the server sample profile.
Published	Status of the server sample profile in the **OMNIS Client/Server system**. Additional information: *(see "Sample profiles – Status", chapter 5.10.5.6, page 269)*
Saved	Time at which the server sample profile was last saved.
Data permissions	Existing data permissions assigned to this server sample profile. **Note**: Applies only if data permissions are enabled and the user has the necessary user rights.

See also

Data permissions – Definition (chapter 4.5.9, page 105)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Publishing the sample profile (chapter 5.10.5.5, page 267)

Sample profiles – Subsection (chapter 5.10.5.1, page 259)

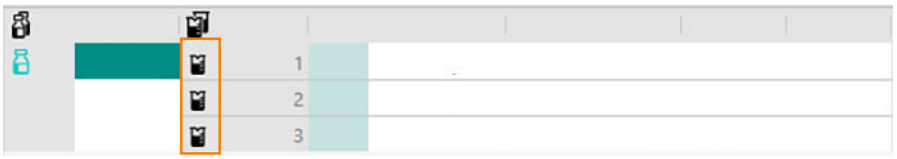
Server sample profile – Definition (chapter 5.10.6, page 270)

5.10.7 Subsamples – Definition

A subsample is a partial quantity of a sample (aliquot or aliquant) that is analyzed in a determination with the help of an operating procedure. A subsample must be created for each determination. Several subsamples of the same sample can be created for multiple determinations.

The run of a determination is defined in the operating procedure that may contain several methods and commands. Data required for performance of the determination can be entered individually for each subsample (e.g. sample size, dilution factor, etc.). Which data are available as subsample data is defined in the properties of the operating procedure.

Example: Three subsamples in the sample list



See also

Editing subsample data (chapter 5.11.1.10.1, page 404)

Recording subsamples (chapter 5.10.7.1, page 273)

5.10.7.1 Recording subsamples

Information on subsamples in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Subsamples can be added automatically to the sample list during a determination using the **ADD TO SAMPLE LIST** command. Additional information: *(see "ADD TO SAMPLE LIST – Properties", chapter 5.11.8.63, page 761)*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

Recording subsamples

Prerequisite:

- A sample list is opened and at the front.
- At least one sample was captured in the sample list: *(see "Recording samples", chapter 5.10.4.1, page 251)*

1 Selecting the sample or subsample

- Click to select the sample under which the new subsample is to be added.
  or
- Click to select the subsample under which the new subsample is to be added.

2 Adding a subsample

- Click on to add a new subsample to the selected sample or subsample. The operating procedure is applied automatically from the preceding subsample.

If a sample profile without operating procedure has been defined, then only one input field (**Subsample name**) and one selection list (**Operating procedure**) are displayed when a subsample is added.

3 Naming or renaming a subsample

- In the **Subsample name** column, double-click in the field and enter the name.
- Confirm the entry with the **[ENTER]** button.

The following characters are not allowed: **. | ' " { }**

4 Changing an operating procedure

- Double-click in the **Operating procedure** field and enter the name of the desired operating procedure or select it from the list.

See also

Editing subsample data (chapter 5.11.1.10.1, page 404)

Operating procedure – Definition (chapter 5.11.1, page 379)

Recording samples (chapter 5.10.4.1, page 251)

Sample list – Overview of functions (chapter 5.10.1.5, page 240)

Sample list – Tab (chapter 5.2.2, page 159)

Starting determination (chapter 5.10.8.6, page 304)

Stopping a determination (chapter 5.10.8.7, page 308)

5.10.7.2 Deleting subsamples

Information on subsamples in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

- *Removing subsamples from the sample list*
- *Deleting subsamples in the sample list*

Removing subsamples from the sample list

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

- A subsample is selected.

1 Removing subsamples

- The following options are available for removing a subsample:
  - Click to remove the selected subsample from the list.
  - Right-click on the selected subsample to open the context menu and select **[Remove from sample list]**.
  - Click the **[DELETE]** key to remove the selected subsample.

Only the selected subsamples are removed when subsamples are removed from the same sample (split samples).

Removed samples and subsamples are removed only from the current sample list, but still continue to be present in the database.

To find removed samples, a search query can be created in the **Samples** work area.

Deleting subsamples in the sample list

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- A sample list is opened and at the front.
- A subsample is selected.

1 Deleting subsamples

- The following options are available for deleting a subsample:
  - Right-click on the selected subsample to open the context menu and select **[Delete]**.
  - Delete the selected subsample with the key combination **[CTRL]**+**[DELETE]**.

Deleted samples and subsamples are deleted permanently from the database and cannot be restored.

See also

Editing subsample data (chapter 5.11.1.10.1, page 404)

Operating procedure – Definition (chapter 5.11.1, page 379)

Recording samples (chapter 5.10.4.1, page 251)

Sample list – Overview of functions (chapter 5.10.1.5, page 240)

Sample list – Tab (chapter 5.2.2, page 159)

Starting determination (chapter 5.10.8.6, page 304)

Stopping a determination (chapter 5.10.8.7, page 308)

5.10.7.3 Subsamples – Statuses

Each subsample has a status, which is displayed as a combination of background color and icon in the status field. Certain statuses can be modified by clicking on the status field and selecting a new status in the context menu. Only the changes which are possible for the current status are displayed in the context menu.

With multiple selected subsamples, all of the status changes which are possible for at least one of the selected subsamples are displayed. If a status change is selected, then this will have an effect only on the subsamples for which this is possible.

Table 1 Statuses of subsamples

Status field	Meaning	Possible status changes
	Ready The subsample is ready for execution. The determination can be started.	Add to running sample series
	Pending execution The determination has been started, but the subsample is not yet analyzed.	Remove from running sample series
	Running The subsample is currently being analyzed.	Hold determination Stop determination
	Work system ready The work system used for the subsample is in the status **Conditioning OK**.	No status change possible
	Work system not ready The work system used for the subsample has **Conditioning not OK** status.	No status change possible
	Held The analysis of the subsample has been paused.	Continue determination Stop determination

Status field	Meaning	Possible status changes
	Waiting for user action The analysis of the subsample has been paused. Execution continues as soon as the displayed instructions in the **Live data** subsection of the **Curves and data** area have been followed by the user.	Hold determination Stop determination
	Waiting for work system The analysis of the subsample has been paused. The work system required for the determination is currently occupied or faulty.	Remove from running sample series
	Completed The analysis of the subsample was successfully completed.	No status change possible
	Canceled after error An error occurred during the analysis of the subsample. The system has ended the determination.	Reset to status "Ready"
	Canceled after stop The user has canceled the analysis of the subsample.	Reset to status "Ready"
	Edited The data of the analysis was modified and saved retroactively.	No status change possible
	Reprocessed, not saved The data of the analysis was modified retroactively, but not yet saved.	No status change possible
	Planned determination The determination of the subsample was planned by **Start planning** and will be started at a defined time. If determinations in the sample list are already being executed at the planned time, then the subsample will be added to the ongoing sample series.	Remove a plan

Status warning for subsamples

A status warning is displayed with the following errors.

Status field	Meaning
	The following errors are signaled with this status warning. Additional information on the errors is displayed when the cursor is moved over the status warning. ▪ **Error during the run test**: The conditions for successful execution of the subsample were not met. Additional information: *(see "Run test – Brief description", chapter 5.10.8.1, page 295)*. ▪ **Boundary violations for results monitoring**: The value of the results or variables lies outside of the defined upper and lower warning limits or control limits. The monitored results are marked under **Results** ▶ **Monitoring** by different status icons ( ). Additional information: *(see "Result monitoring – Status", chapter 5.10.13.4.1, page 355)*. ▪ **Model outliers**: At least one result of the subsample is outside the defined limits or could not be identified or verified. The results concerned are marked under **Results** ▶ **Predictions** in the tables of the **Overview** and **Reprocessing** areas by the status icon. Additional information: *(see "Reprocessing predictions", chapter 5.10.13.5.1, page 363)*.

The status warning is updated when a new run test is carried out or when the results are recalculated.

Synchronization status of subsamples

In the **OMNIS Client/Server system**, every subsample has an additional status that shows the status of the synchronization with the OMNIS Server.

Status field	Meaning
No status display	**Not saved or is not synchronized.** The subsample was not uploaded to the OMNIS Server. Either the sample list has not been saved yet or the subsample does not meet the conditions for synchronization: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*
	Subsample synchronized The subsample has been synchronized with the OMNIS Server.
	Subsample in synchronization The subsample is currently being synchronized with the OMNIS Server.
	Synchronization has been paused The synchronization of the subsample has been paused. The synchronization will be resumed automatically as soon as the sample list is saved or the current determination is ended.
	Not synchronized The subsample cannot be synchronized with the OMNIS Server because the connection is interrupted. The subsample will be synchronized automatically once the connection is restored.
	Synchronization failed The subsample cannot be synchronized with the OMNIS Server because an unknown error occurred. Contact your regional Metrohm representative.

See also

Editing sample list (chapter 5.10.1.2, page 212)

Pausing determination (chapter 5.10.8.8, page 309)

Predictions – Subsection (chapter 5.10.13.5, page 359)

Sample list – Tab (chapter 5.2.2, page 159)

5.10.7.4 Recording weighing data

If a balance is connected to the OMNIS system, then the weight and the weighing unit can be applied directly into a sample list. A weight and the corresponding unit can be added to the subsample data with a **WEIGH** command, a **REQUEST** command or directly by pressing the **[Print]** key on the balance.

The following options for recording weighing data are available in the OMNIS Software:

(see "Editing subsample data", chapter 5.11.1.10.1, page 404)

- *Applying weighing data directly*
- *Applying weighing data with a WEIGH command*
- *Applying weighing data by weighing by difference*

Balances of the **Cubis II** series from Sartorius come with automatic configuration and additional features. These are not described in this manual. Detailed instructions for connecting and operating devices of the **Cubis II Balance** type can be found here: *(see "Operating the Cubis II Balance", chapter 5.12.2.12.2, page 886)*

Applying weighing data directly

Prerequisite:

- The balance is connected to the computer via the RS-232-interface or via the local Ethernet network.
- The balance was configured in the OMNIS system under **Equipment ▶ Inventory ▶ Other instruments**:*(see "Configuring the balance", chapter 5.12.2.12.1, page 884)*

1 Selecting subsample

In the sample list, select a subsample that exhibits an input field of the **Sample size** type and that is to receive weighing data.

2 Weighing in a subsample

Weigh in the subsample at the balance.

3 Pressing Print key

On the balance, press the **[Print]** key.

Carrying over weighing data with the WEIGH command

Prerequisite:

- The balance is connected to the computer via the RS-232-interface or via the local Ethernet network.
- The balance was configured in the OMNIS system under **Equipment ► Inventory ► Other instruments**:*(see "Configuring the balance", chapter 5.12.2.12.1, page 884)*
- An input field of the **Result** type must be defined for the result in the parameters of the operating procedure.

1 Compiling method

Create a method with a **WEIGH** command and a **CALC** command.

2 Applying unit and weight

To apply the unit in the parameters of the **CALC** command, make the following entries:

- Select the '**Unit.Result.***Command name*' variable in the **Result unit** field under **Formula ► Command variables**.

To apply the weight in the parameters of the **CALC** command, make the following entries:

- Select the '**Weight.Result**.*Command name*' variable in the **Formula** field under **Command variables**.
- Select the '*Variable name*.**CurrentSubsampleData**' variable in the **Save result in variable** field under **Subsample data**.

3 Starting determination

Start the determination.

The OMNIS Software confirms the receipt of the weighing data with an acoustic signal. Should it not be possible to enter the weight and the unit in the input fields of the selected subsample, then this will also be confirmed by an acoustic signal.

Applying weighing data by weighing by difference

Prerequisite:

- The balance is connected to the computer via the RS-232-interface or via the local Ethernet network.
- The balance was configured in the OMNIS system under **Equipment ► Inventory ► Other instruments**:*(see "Configuring the balance", chapter 5.12.2.12.1, page 884)*
- An input field of the **Sample size** type must be defined in the parameters of the operating procedure.
- The subsample must be in execution with a **REQUEST** command and the **REQUEST** pop-up window must be open.

- The weighing data can be changed as long as the **REQUEST** pop-up window is open. It can subsequently be changed only if the **Editable field** option was activated when the input field was defined in the operating procedure.

1 Changing unit

To change the unit, activate the check box **Edit unit** in the parameters of the **REQUEST** command.

2 Weighing the subsample and taring the balance

Weigh the subsample at the balance and then tare the balance.

3 Adding sample

Once the **REQUEST** command is displayed, add the sample and place the empty weighing vessel back on the balance.

4 Pressing Print key

On the balance, press the **[Print]** key.

5 Applying values of the subsamples

Adopt the values for the current subsample by clicking on **[Continue]**.

The values for the running subsample are adopted.

The adoption of the weighing data works only if the sample list is open and the **REQUEST** pop-up window is open. The data sent by the balance is not adopted if another work area or another tab in the **Samples** work area is open.

Behavior in the Audit Trail

If the Audit Trail is activated for the OMNIS system, all actions are recorded via the application on the balance as follows:

- Both a successful login with a **REQUEST** command and the weighing-in of a subsample result in a further entry in the Audit Trail, in which additional information about the balance is recorded:
  - Serial number of the balance
  - Display name of the balance in the OMNIS Software

See also

Configuring the balance (chapter 5.12.2.12.1, page 884)

Editing subsample data (chapter 5.11.1.10.1, page 404)

REQUEST – Parameters (chapter 5.11.8.77, page 794)

5.10.7.5 Reprocessing subsample data

After the determination of a subsample has been performed, the sample data or subsample data can be reprocessed directly in the sample list. This means that erroneous entries can be corrected.

Sample data and subsample data that are used as **Result** cannot be changed retroactively.

Prerequisites:

- The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.
- The desired determination has finished.

1 Marking the field

- Select the subsample that you want to reprocess.
- Double-click in the field for which you want to reprocess the content.

Only fields that were defined as **editable** in the parameters of the operating procedure can be reprocessed. Fields for dates and numbers and texts that are used as a result are never editable.

The content of the field is marked in a color and can be edited.

2 Entering the change

- Enter the desired content.
- Confirm the entry with **[Enter]**.

The reprocessed subsample is marked with .

3 Saving the change

- Save the sample list by clicking on .

The reprocessed subsample is marked with .

See also

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Recording subsamples (chapter 5.10.7.1, page 273)

Reprocessing calculations (chapter 5.10.13.1.1, page 350)

Subsamples – Statuses (chapter 5.10.7.3, page 276)

5.10.7.6 Preparing a CSV file

In the OMNIS Software, CSV files can be used to import and export subsample data (e.g. sample lists from a third-party system).

Preparing a CSV file for import

1 Opening a CSV file

- Open the CSV file with sample data and subsample data from the third-party system in a table editing program.
- Format the data as a table. Use a **semicolon** as a separator.

Example of a CSV file with sample data and subsample data: *Metrohm Knowledge Base*

SP Example 1;mySample;1;text example;mySubsample 1;OP Example 1;2;Text 1;1;;
;;1;text example;mySubsample 2;OP Example 1;2;Text 2;2;;
;;1;text example;mySubsample 3;OP Example 1;2;Text 3;;;
;;1;text example;mySubsample 4;OP Example 1;2;Text 4;4;;
;;1;text example;mySubsample 5;OP Example 1;2;Text 5;5;;
SP Example 2;mySample;2;text example;another text example;mySubsample 1;OP Example 2;3;Text 1;1;1
;;2;text example;another text example;mySubsample 2;OP Example 2;3;Text 2;2;2
;;2;text example;another text example;mySubsample 3;OP Example 2;3;Text 3;;
;;2;text example;another text example;mySubsample 4;OP Example 2;3;Text 4;4;4
;;2;text example;another text example;mySubsample 5;OP Example 2;3;Text 5;5;5
;;2;text example;another text example;mySubsample 6;OP Example 2;3;Text 6;3;3
;;2;text example;another text example;mySubsample 7;OP Example 2;3;Text 7;1;1
;;2;text example;another text example;mySubsample 8;OP Example 2;3;Text 8;3;3
;;2;text example;another text example;mySubsample 9;OP Example 2;3;Text 9;5;5
;;2;text example;another text example;mySubsample 10;OP Example 2;3;Text 10;1;1

2 Creating an operating procedure in OMNIS Software

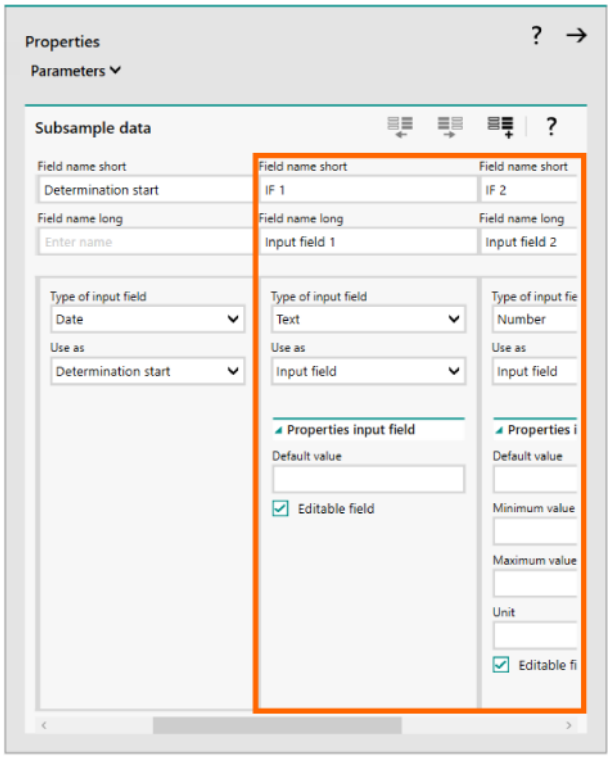
- Create a new operating procedure under **Processes** ▶ **Operating procedures**.
- Enter the name of the operating procedure that must match the name in the CSV file in **Properties** ▶ **General**.

Additional information on creating an operating procedure: *(see "Creating and editing an operating procedure", chapter 5.11.1.3, page 387)*

3 Defining subsample data

- Define the required number of input fields for the subsample data in the operating procedure under **Properties** ▶ **Parameters**. Ensure the following:
  - The type of input field is defined as **Text**, **Number** or **Date** according to the data in the CSV file.
  - The **Editable field** check box is enabled.

SP Example 1	mySample	1	text example	mySubsample 1	OP Example 1	2	Text 1	1		
				mySubsample 2	OP Example 1	2	Text 2	2		
				mySubsample 3	OP Example 1	2	Text 3			
				mySubsample 4	OP Example 1	2	Text 4	4		
				mySubsample 5	OP Example 1	2	Text 5	5		
SP Example 2	mySample	2	text example	another text example	mySubsample 1	OP Example 2	3	Text 1	1	1
					mySubsample 2	OP Example 2	3	Text 2	2	2
					mySubsample 3	OP Example 2	3	Text 3		
					mySubsample 4	OP Example 2	3	Text 4	4	4
					mySubsample 5	OP Example 2	3	Text 5	5	5
					mySubsample 6	OP Example 2	3	Text 6	3	3
					mySubsample 7	OP Example 2	3	Text 7	1	1
					mySubsample 8	OP Example 2	3	Text 8	3	3
					mySubsample 9	OP Example 2	3	Text 9	5	5
					mySubsample 10	OP Example 2	3	Text 10	1	1



If a cell in the column for the subsample data in the CSV file remains empty, then the default value, which is defined in the subsample data of the operating procedure under **Subsample data** ▶ **Properties input field**, is entered automatically when the file is imported.

Only input fields need to be considered in the CSV file. Fields for results (e.g. determination start) must be ignored and must not be written as empty cells in the CSV file.

4 Creating a sample profile in OMNIS Software

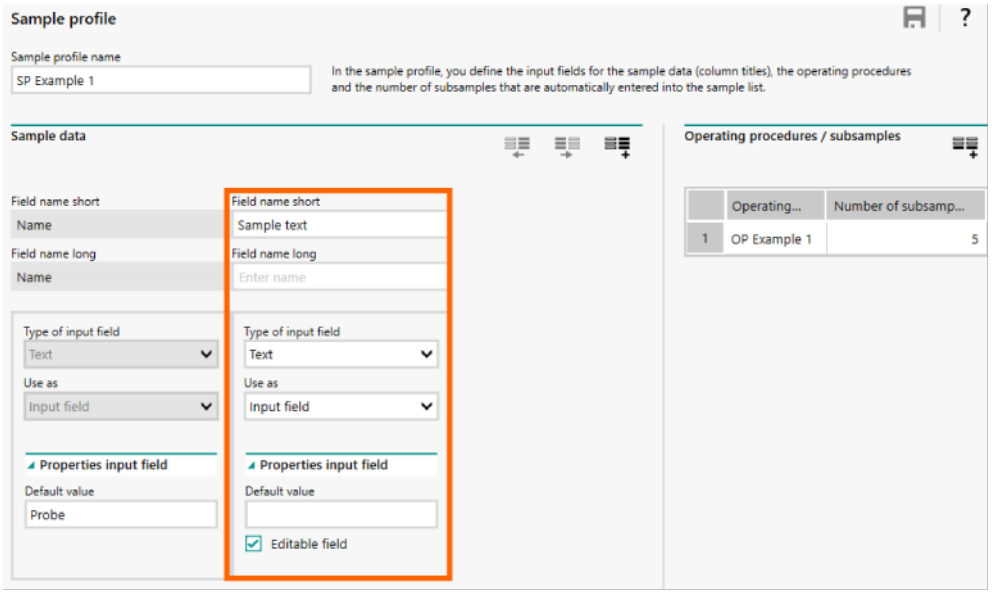
- Create a new sample profile under **Samples** ▶ **Sample profiles**.
- Enter the name of the sample profile in the **Name of the sample profile** field that must match the name in the CSV file.

Additional information on creating a sample profile: *(see "Creating and editing sample profile", chapter 5.10.5.2, page 261)*

5 Defining sample data

- Define the required number of input fields for the sample data under **Sample profile** ▶ **Sample data**. Ensure the following:
  - The type of input field is defined as **Text**, **Number** or **Date** according to the data in the CSV file.
  - The **Editable field** check box is enabled.
- Define the operating procedure and the required number of subsamples under **Sample profile** ▶ **Operating procedures / subsamples**. The operating procedure must match the operating procedure in the CSV file.

SP Example 1	mySample	1	text example	mySubsample 1	OP Example 1	2	Text 1	1		
				mySubsample 2	OP Example 1	2	Text 2	2		
				mySubsample 3	OP Example 1	2	Text 3			
				mySubsample 4	OP Example 1	2	Text 4	4		
				mySubsample 5	OP Example 1	2	Text 5	5		
SP Example 2	mySample	2	text example	another text example	mySubsample 1	OP Example 2	3	Text 1	1	1
					mySubsample 2	OP Example 2	3	Text 2	2	2
					mySubsample 3	OP Example 2	3	Text 3		
					mySubsample 4	OP Example 2	3	Text 4	4	4
					mySubsample 5	OP Example 2	3	Text 5	5	5
					mySubsample 6	OP Example 2	3	Text 6	3	3
					mySubsample 7	OP Example 2	3	Text 7	1	1
					mySubsample 8	OP Example 2	3	Text 8	3	3
					mySubsample 9	OP Example 2	3	Text 9	5	5
					mySubsample 10	OP Example 2	3	Text 10	1	1

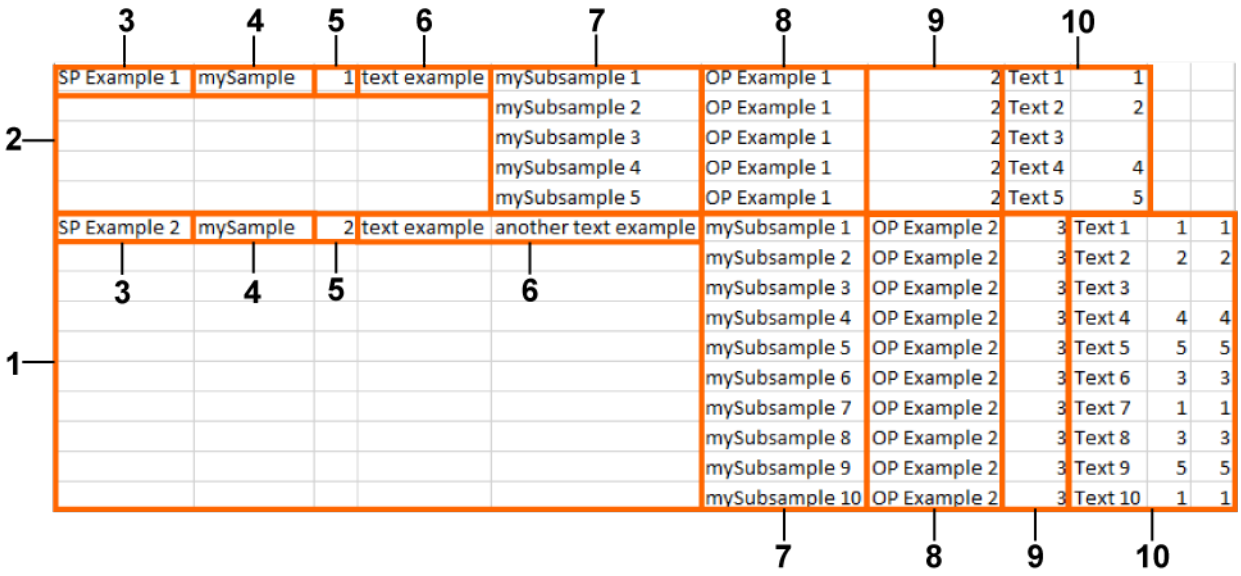


6 Saving the CSV file

- Click on **[Save]** in the table editing program.
  Select the required memory location.
- Select the **CSV UFT-8 (Comma delimited)** format as the **File type**. Make sure that the correct separators are used.
- Create the CSV file by clicking on **[Save]**.

Parts of a CSV file

A correctly created CSV file can appear in Excel as follows:



1 **Sample 1**

2 **Sample 2**

3 **Name of the sample profile**
Sample profile created with identical name in the OMNIS Software.

4 **Sample name**
Self-defined sample name. The following characters are not allowed in the sample name: **. | ' " { }**

5 **Number of additional sample data**
The maximum number of sample data must not exceed the number of sample data in the sample profile.

If there are fewer fields defined for sample data in the CSV file than are designated in the sample profile, then the sample data in the sample list is filled from left to right.

6 **Content of the sample data**
Type of sample data field defined in the sample profile. Only input fields need to be considered in the CSV file.

7 **Subsample names**
Self-defined subsample name. The following characters are not allowed: **. | ' " { }**

8 **Name of the operating procedure**
Operating procedure created with identical name in the OMNIS Software.

9 **Number of additional subsample data**
The maximum number of subsample data must not exceed the number of subsample data in the sample profile.

If there are fewer fields defined for subsample data in the CSV file than are designated in the operating procedure, then the subsample data in the sample list is filled from left to right.

10 **Content of the subsample data**
Type of subsample data field defined in the operating procedure. Only input fields need to be considered in the CSV file.

Preparing for export

The decimal separator for the OMNIS Software interface (e.g. in the **Raw data** area) is taken from the Windows settings. When exporting to a CSV file, this decimal separator is also adopted. To ensure that the desired decimal separator is used, individual options in the Windows system settings may have to be changed.

These instructions apply for Windows 11.

1 Changing the regional format

- Navigate to the Windows start menu and open the settings.
- Open the **Time & Language** area in the settings.
- In the **Region** menu item under **Regional format**, select an option from the selection list that uses a period as decimal separator (e.g. **English (United States)**).

2 Changing the decimal separator separately

- Navigate to the Windows start menu and open the Control Panel.
- Open the **Clock & Region** area in the Control Panel.
- In the **Region** menu item, open the **Change date, time, or number formats** option.
- In the **Region** Explorer window, click on the **Additional settings** button.
- Select or enter the required character under **Decimal symbol**.
- Click on **[OK]** and return to the **Region** Explorer window.

3 Saving changes

- In the **Region** Explorer window, open the **Administrative** tab.
- Click on the **Copy settings** button.
- Activate the check box for **Welcome screen and system accounts** and **New user accounts**.
- Close all the programs and restart the computer.

See also

Editing subsample data (chapter 5.11.1.10.1, page 404)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

5.10.7.7 Importing subsample data

There are 2 options in the OMNIS Software for importing sample data and subsample data:

- *(see "Importing a sample data file", page 290)* containing sample data and subsample data from the OMNIS Software.

- *(see "Importing a CSV file", page 290)* containing sample data and subsample data from a third-party system.

Importing a sample data file

Prerequisite:

- A sample list is opened and at the front.
- At least one OMNIS sample data file (***.osin**) is available.
- The user has the necessary rights. Further information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting sample data and subsample data

- Click on to open the **Import sample data and subsample data** window in **Samples** ▶ **Sample list**.

2 Browsing for folder

- Select the folder in which the desired subsample data is saved.

3 Selecting the file type

- Select the ***.osin** file type at the bottom right of the window.
- Select the OMNIS subsample data file or enter the name of the OMNIS subsample data file in the **File name** field.

4 Confirming and importing the selection

- Click **[Open]** to confirm the selection.

The sample data and subsample data from the file are imported into the opened sample list.

Importing a CSV file

Prerequisite:

- The CSV file is prepared according to the instructions: *(see "Preparing a CSV file", chapter 5.10.7.6, page 284)*
- The sample profile listed in the CSV file exists under the identical name in the OMNIS Software.
- The number and name of the fields in the sample data of the sample profile match the number and name of the sample data in the CSV file.
- The operating procedure listed in the CSV file exists under the identical name in the OMNIS Software.
- The number and name of the fields in the subsample data of the operating procedure match the number and name of the subsample data in the CSV file.

- The data in the CSV file has no column header.
- A sample list is opened and at the front.
- The user has the necessary rights. Further information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting sample data and subsample data

- Click on to open the **Import sample data and subsample data** window in **Samples** ▶ **Sample list**.

2 Browsing for folder

- Select the folder in which the desired CSV file is saved.

3 Selecting the file type

- Select the ***.csv** file type at the bottom right of the window.
- Select the CSV file or enter the name of the CSV file in the **File name** field.

4 Confirming and importing the selection

- Click **[Open]** to confirm the selection.

The sample data and subsample data from the CSV file are imported into the opened sample list.

See also

Editing subsample data (chapter 5.11.1.10.1, page 404)

Exporting subsample data (chapter 5.10.1.3, page 220)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Subsample data – Definition (chapter 5.11.1.10, page 403)

5.10.7.8 Sending data to third-party software

Data can be exchanged between OMNIS Software and third-party software via a **web API**. After configuring this interface and performing necessary prerequisites for secure data exchange, third-party providers can use the OMNIS Software and send sample data and subsample data to the OMNIS system. In turn, data can also be sent from the OMNIS Software to self-defined interfaces.

Information on configuring the web API: *3rd Party Data Integration API – Technical White Paper*

Further information on the data exchange between the OMNIS Software and third party software: *(see "Data exchange with third-party software – Definition", chapter 4.9, page 147)*

There are 3 options in the OMNIS Software for sending subsample data:

- *Automatic sending* during a determination with the **CALL WEB API** command: *(see "CALL WEB API - Parameter", chapter 5.11.8.65, page 771)*
- *Automatic sending* after expiration of a determination
- *Manual sending* from the sample list

Automatic send from the operating procedure

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Further information: *Metrohm Knowledge Base*
- User management is activated.

1 Opening an operating procedure

- In **Processes** ▶ **Operating procedures**, select the required operating procedure and open it with a double-click.

2 Opening web exports

- Click on to open the **Properties** window.
  or
- Double-click on

to open the **Properties** window directly.

The web exports can be defined in **Properties** ▶ **Web exports**.

3 Adding a web export

- Click on to add a new web export.

4 Defining a web export

- In the **API endpoint URL** field, enter the web address to which the web export will be sent.
- Open the **Request Body for web export** editor by clicking on **[Edit Request Body]**. The Request Body can be defined using formulas in this window.

  Click on the f_x to open the formula editor.
- Select the **authentication type** and, if necessary, fill in the displayed parameters.

5 Saving a web export

- Save the parameters by clicking on .

After post-editing the samples in the sample list, the data must be sent manually once again.

Automatic send with the CALL WEB API command

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Further information: *Metrohm Knowledge Base*
- User management is activated.

1 Inserting a command

- Use drag and drop to insert the **CALL WEB API** command from the Library into the operating procedure in **Processes** ▶ **Operating procedures**.

With the **CALL WEB API** command, it cannot be guaranteed that all determination results are already available and can be sent. For a complete web export, a web export definition must be made in the properties of the operating procedure.
In addition to sending subsample data, the **CALL WEB API** command can also be used to actuate any web APIs using the **POST** HTTP method. Thus, the command can also be used for laboratory automation.

2 Opening the parameters

- Click on to open the **Properties** window.
  or
- Double-click on the **CALL WEB API** command to open the **Properties** window directly.

The web exports can be defined in **Properties** ▶ **Parameters**.

3 Defining a web export

- Define the parameters for the command: *(see "CALL WEB API - Parameter", chapter 5.11.8.65, page 771)*

4 Saving a command

- Save the parameters by clicking on .

Manual send from the sample list

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Further information: *Metrohm Knowledge Base*
- User management is activated.
- The sample list is open.
- The data in the sample list has been saved.
- The subsamples to be exported were executed with an operating procedure for which a web export was defined.

1 Selecting samples and subsamples

- Click on or to select individual samples or subsamples.
  or
- Click on or to select all samples or subsamples of a group.
- To select multiple samples or subsamples, select the required samples or subsamples while pressing down the **[SHIFT]** key or the **[CTRL]** key.

2 Sending data

- Click on to open the **Export data** window.
- Select the option **Web export** from the selection list in the **Export type** field.
- Select the option **Selected subsamples with web export** or **All subsamples in the list with web export**.
- Create the web export by clicking on **[Export]**.

The data of the selected subsamples, which were executed with an operating procedure with web export definition, are sent to the web API once again.

If the version of the operating procedure associated with the subsample is not the latest version, any changes to the web export definition will be applied when the data is resent. The data is sent with the web export definition in the latest version of the operating procedure.

If there are unsaved changes in the sample list, a message will appear asking if the web export is to be performed anyway.

See also

CALL WEB API - Parameter (chapter 5.11.8.65, page 771)

Operating procedure – Properties (chapter 5.11.1.2, page 383)

5.10.8 Determination – Definition

A determination comprises the preparation, analysis and evaluation of a subsample. All available sample lists are displayed in **Samples** ▶ **Sample lists**. A new tab opens when a sample list is double-clicked. Determinations can be performed and modified here.

Distinction is made between the following determination runs:

- Single determination
- Series determination
- Parallel determination

See also

Parallel determination – Run (chapter 5.10.8.4, page 299)

Pausing determination (chapter 5.10.8.8, page 309)

Series determination – Run (chapter 5.10.8.3, page 298)

Single determination – Run (chapter 5.10.8.2, page 297)

Starting determination (chapter 5.10.8.6, page 304)

Stopping a determination (chapter 5.10.8.7, page 308)

Subsamples – Statuses (chapter 5.10.7.3, page 276)

5.10.8.1 Run test – Brief description

In the OMNIS Software, there are 3 types of run test: **Manual run test**, **Automatic run test** and **Preliminary run test.**

The **Manual run test** is triggered by clicking on . This test checks all subsamples from the sample list in the **Ready** status one after the other.

The **automatic run test** is always carried out when a run is started by clicking on or . This test is carried out before the determination of each subsample and checks whether all conditions have been fulfilled for successfully executing the selected subsamples. If the **automatic run**

test is successful, then the subsample is carried out without feedback. Then the next subsample is checked.

The **preliminary run test** is carried out enabled before the start of a determination after clicking on or ,, if the **Include preliminary run test** check box in **Settings** ▶ **General settings** is enabled. This test checks all selected subsamples together before starting a determination. If the preliminary run test is successful, then the determination is started. As the **automatic run test** is included in each determination, the **automatic run test** is then carried out before the determination of each subsample.

A run test can be carried out only if the sample list contains subsamples that have not yet been analyzed.
Only the selected subsample is checked in a single determination.

Each run test carries out the following points:

Checking user rights

- The appropriate user rights for executing a determination must be assigned.

Checking instrument licenses

- The number of instrument licenses is checked.

Loading the sample data

- The sample data entered for a determination is loaded.

Checking the validity of the sample data and subsample data

- The entered data must correspond to the defined method variables and be valid.
- The subsample data must have been entered correctly in the operating procedure.

- If the subsample data has been changed, the run test must be carried out once again.
- Subsamples with invalid data can be saved, but not executed.
- Number fields must not be empty. Text fields may be empty.

Checking the methods

- The feasibility of the methods is checked.
- All commands used must have correct parameters.
- A functional unit must be assigned to all instrument-dependent commands.

Check the expiry date of the equipment

- The **Working life**, **Validity period** or **limit** of equipment is checked. If the equipment has expired, a prompt appears to replace the expired equipment or to execute a new calibration or titer determination.

If the **Prevent determination with expired equipment** function is enabled in the operating procedure under **Properties** ▶ **Execute with**, then the determination can be continued only if the user has been assigned the **Start determinations with expired equipment** user right. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

Checking the compatibility of equipment

- The equipment to be used must comply with the defined solution conditions and sensor conditions.

Checking the model

- The following models used in the **PREDICT** command are checked:
  - Checking quantification models and their slope/y-intercept corrections
  - Identification models
  - Model hierarchies

The models and also the assigned slope/y-intercept corrections of the model hierarchy are also checked during the run test of the model hierarchies.

Assigning a determination ID

- A unique determination ID is assigned for each determination.

See also

Creating and deleting sample lists (chapter 5.10.1.1, page 211)

Editing sample list (chapter 5.10.1.2, page 212)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Sample list – Tab (chapter 5.2.2, page 159)

5.10.8.2 Single determination – Run

The subsample selected in the sample list is analyzed individually in a single determination. The system executes the following steps after the start of the single determination:

1 – Executing the automatic run test

The automatic run test checks whether the determination can be run.

If the automatic run test discovers an error, then an error message will appear and the determination will not be started. The error described in the message must be eliminated.

2 – Reserving functional units

If the automatic run test was performed successfully, then the determination is started.

First, the functional units of the assigned work system will be reserved for the run. If more than one work system is assigned to a method, the OMNIS Software reserves the first suitable work system and its functional units for the run.

3 – Executing the operating procedure

Once the functional units have been reserved, the determination is executed according to the operating procedure.

See also

Run test – Brief description (chapter 5.10.8.1, page 295)

5.10.8.3 Series determination – Run

In a series determination, all subsamples in the sample list are analyzed in sequence. The system executes the following steps after the start of the series determination:

1 – Reserving subsamples

All executable subsamples of the sample list receive the status **Pending execution** (orange status field) and can no longer be edited.

The sample list is then run through from top to bottom. The steps **2** to **4** are carried out for each subsample.

2 – Executing the automatic run test

The automatic run test checks whether the determination can be run.

If the automatic run test discovers an error, then an error message will appear and the determination will not be started. The error described in the message must be eliminated.

3 – Reserving functional units

If the automatic run test was performed successfully, then the determination is started.

First, the functional units of the assigned work system will be reserved for the run. If more than one work system is assigned to a method, the OMNIS Software reserves the first suitable work system and its functional units for the run.

When starting the determination, if the work system is reserved by another ongoing determination, the system waits until the required work system is available again. Then the run is resumed.

4 – Executing the operating procedure

Once the functional units have been reserved, the determination is executed according to the operating procedure.

If an error occurs during an ongoing series determination, then the series determination is stopped. The status of the subsamples that have not yet been analyzed will be reset to **Ready** (light-green status field).

See also

Run test – Brief description (chapter 5.10.8.1, page 295)

5.10.8.4 Parallel determination – Run

To be able to execute parallel determinations, at least the **2 Parallel Titrations** function license must be activated.

Further information on the respective license version can be obtained at *http://www.metrohm.com* or from your regional Metrohm representative.

Further information on the activation of function licenses: *(see "Activating the function license", chapter 4.2.3, page 35)*

The subsamples are analyzed simultaneously wherever possible in a parallel determination. The determinations of several subsamples are started shortly after each other and executed simultaneously. The system executes the following steps after the start of the parallel determination:

1 – Reserving subsamples

All executable subsamples of the sample list receive the status **Pending execution** (orange status field) and can no longer be edited.

The sample list is then run through from top to bottom and up to 4 determinations of subsamples can be carried out simultaneously. The steps **2** to **4** are carried out for each subsample.

2 – Executing the automatic run test

At the start of the analysis of each subsample, the automatic run test checks whether the determination can be run.

If the automatic run test finds an error, then an error message appears. The error described in the message must be eliminated before the run of the parallel determination has been completed. After that, subsamples that contain an error can be reset to the status **Ready** (light-green status field) or, alternatively, new subsamples can be created.

If an optional run of the **Execute on error** type is used in the operating procedure, then behavior in case of an error can be defined there.

3 – Reserving functional units

The determination is started as soon as the automatic run test has been performed successfully. By default, the functional units of all the work systems assigned are reserved at the start of the determination. If more than one work system is assigned to a method, the OMNIS Software reserves the first suitable work system and its functional units for the run.

When starting the determination, if the work system is reserved by another ongoing determination, the OMNIS Software waits until the required work system is available again. Then the run is resumed.

The following 2 options are available to change the reservation behavior:

- To reserve work systems only when they are needed by a method, the **Reserve work systems only when needed** check box can be enabled under **Properties** ▶ **Execute with** in the operating procedure.
- To release a reserved work system directly after a method has ended, the method can be selected in the operating procedure and the **Release work system after completing the method** check box enabled under **Properties** ▶ **Execute with**.

Additional information on the user-defined reservation behavior:
(see "Configuring a parallel determination", chapter 5.10.8.5, page 301)

4 – Executing the operating procedure

Once the functional units have been reserved, the determination is executed according to the operating procedure. The system proceeds as follows as soon as a method is completed and the assigned work system is available once again:

- The system checks if the work system required for the next method in the operating procedure is available. If it is available, the method is started.
- The system goes through the sample list once again from top to bottom and checks whether the work system can be used for a waiting subsample. The first subsample that fulfills this criterion is started.

If the **Prevent determination with expired equipment** check box at **Processes** ▶ **Operating procedures** in the operating procedure in **Properties** ▶ **Execute with** is enabled, then this only applies to the selected operating procedure. If several work systems have been assigned to an operating procedure, then the determination of the subsamples is canceled as soon as a work system with expired equipment is used.

In case of frequent errors during parallel determination: *(see "Configuring a parallel determination", chapter 5.10.8.5, page 301)*

See also

Activating the function license (chapter 4.2.3, page 35)

Configuring a parallel determination (chapter 5.10.8.5, page 301)

Operating procedure – Properties (chapter 5.11.1.2, page 383)

Run test – Brief description (chapter 5.10.8.1, page 295)

5.10.8.5 Configuring a parallel determination

The subsamples are analyzed simultaneously wherever possible in a parallel determination. The determinations of several subsamples are started shortly after each other and executed simultaneously. Due to the complexity of the run, a few points must be taken into account during the configuration of a parallel determination.

User-defined reservation behavior

All work systems are reserved at the start of determination and released at the end by default. The following 2 options are available to change the reservation behavior:

- **Release work system after completing the method** check box in the properties of the method under **Execute with**
  With this, the work system that was reserved by the method is released as soon as the method is completed. It can then be used for the analysis of other subsamples. If it is needed again for the previous analysis, then it will be reserved again.
- **Reserve work systems only when needed** check box in the properties of the operating procedure under **Execute with**
  With this, selected work systems are only reserved during the run of the determination once they are needed for the method. With this, a determination can already be started, even if some functional units of these selected work systems are still reserved by other determinations.

By activating a user-defined reservation behavior, a **deadlock** may occur between subsamples. This is caused by interdependencies between subsamples, e.g. if a functional unit is needed for the analysis of subsample 1, which has already been reserved for the analysis of subsample 2. At the

same time, a functional unit is needed for the analysis of subsample 2, which is still reserved for the analysis of subsample 1. At this point, both subsamples are blocked. The system cancels the analysis of one of the subsample with an error.

In order to prevent such interdependencies, the following steps need to be taken into account when configuring operating procedures:

1. Assemble a work system that only contains those functional units that urgently need to be released after the end of the method, since they are needed for another method. The number of these functional units to be released should be kept as low as possible.

   The **Main Module Pick&Place** does not need to be released prematurely, as it is shared between the subsamples.

2. Functional units that are released prematurely are not to be used in the same operating procedure again, if possible. If this cannot be avoided, then the functional units always need to be reserved or released for a method simultaneously.

3. If different operating procedures are used in the parallel determination, they should have a similar order for reserving, using, releasing and reserving a work system again, if possible to avoid a deadlock.

The reservation behavior can be further configured with the **Skip optional runs (error/stop) with a new reservation of work systems** check box under **Properties** ► **Execute with**. By activating the check box, the run sequences **Execute on error** and **Execute on stop** are skipped if they would reserve a work system that has already been released. This avoids that the defined behavior in case of an error or stop is executed for a work system that has already been released and is being used in another run. If enabled, this setting applies for all run sequences of this type within the separate methods, but also within the entire operating procedure.

Continuing a determination after an error

If an error occurs while a parallel determination is running, then the analysis of the affected subsample will be canceled. The subsample is in the **Canceled after error** status. All other subsamples that require the faulty work system have the status **Waiting for work system**.

To continue the determination of the canceled and stopped subsamples, the following steps must be performed:

Prerequisite:

- The affected sample list is opened and at the front.

1 For error in work system

- Eliminate the cause of the error. If necessary, remove beakers that are still on the workstation.
- If the affected sample can still be used, place it back on the sample rack.
- Initialize the affected instrument or the functional unit if necessary.

2 For error in operating procedure

- Check whether the assignment of the work system within the operating procedure complies with the recommendations mentioned above.

3 Ending running determinations after a time delay (optional)

- End the ongoing determinations by clicking on .

With parallel determinations, the system continuously checks whether the work system is available again for all samples with **Waiting for work system** status, one after the other. After initialization, the determination is automatically continued for the sample that is currently being checked. To avoid this, the **End determinations with a time delay** function is recommended.

4 Determining the canceled subsample once again

- Click on the status field of the subsample with the **Canceled after error** status to open the context menu. Click on to reset the subsample to the **Ready** status.
- **If step 3 was not performed:** Click on the status field of the subsample to open the context menu and click on there to add the selected subsample to the running parallel determination.

  Or click on to add all executable subsamples in the sample list to the running parallel determination.
- **If step 3 was performed:** Click on or to start the parallel determination.

See also

Activating the function license (chapter 4.2.3, page 35)

Operating procedure – Properties (chapter 5.11.1.2, page 383)

Parallel determination – Run (chapter 5.10.8.4, page 299)

Run test – Brief description (chapter 5.10.8.1, page 295)

5.10.8.6 Starting determination

- *Single determination*
- *Series determination or parallel determination*
- *Add executable subsamples to an ongoing determination*
- *Plan determinations of subsamples*

Only saved subsamples with the **Ready** status can be analyzed. Executable subsamples can be identified by the light green background color in the status field.

The current status of the subsamples is displayed in the sample list: *(see "Subsamples – Statuses", chapter 5.10.7.3, page 276)*

Single determination

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Selecting subsample

- Click on in the sample list to select the required subsample.

2 Starting determination

- Click on to start the determination of the selected subsample.

The operating procedure for the determination of the selected subsample is started. No additional subsample can be added for analysis during a single determination.

If the work system required for a determination is occupied, the determination will not be started until the work system is once again free.

Series determination or parallel determination

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses and function licenses are enabled.
  Additional information: *Metrohm Knowledge Base*

1 Selecting samples or subsamples (optional)

- Click on or in the sample list to select the required sample or subsample.
  or
- Click on in the sample list to select the required sample group.

The number of the selected subsamples is indicated on the button next to the Start icon for the determination.

2 Selecting determination type

- **Series determination**: Select ↓ in the selection list below the sample list.
  The series determination starts with the first executable subsample. This subsample is highlighted in dark green. All executable subsamples of the sample list are then analyzed in sequence. Subsamples can be added to the ongoing analysis during a series determination.
  or
- **Parallel determination**: Select ↓↓ in the selection list below the sample list.
  The parallel determination is started with up to 4 executable subsamples. These subsamples receive the focus and are highlighted in orange. All executable subsamples from the sample list are then analyzed in sequence. Up to 4 subsamples can be in the **Running** status at the same time. The focus switches automatically thereby to the next subsample currently being executed. Subsamples can be added to the ongoing analysis during a parallel determination.

3 Starting determination

- Start the determination for the selected subsamples by clicking on . The remaining number of subsamples still to be determined is displayed on the button and continuously updated during the determination.
  or
- Start the determination for all executable subsamples in the sample list by clicking on . The remaining number of subsamples still to be determined is displayed on the button and continuously updated during the determination.

If the work system required for a determination is occupied, the determination will not be started until the work system is once again free.

If an operating procedure present in the sample list is changed in **Processes** ▶ **Operating procedures** but has not yet been executed, then the latest version of the operating procedure is loaded at the time a determination is started.

Selected subsamples can be removed from a sample series, once that series has already been started. To accomplish this, right-click on the status field of the corresponding subsample to open the context menu and select **Remove from running sample series**. These subsamples are reset again to **Ready**.

Adding executable subsamples to an ongoing determination

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- There are several executable subsamples in the sample list.

1 Starting determinations

- Use ▶ to start the determinations of the selected samples and subsamples.

2 Adding single executable subsamples to an ongoing determination

- Right-click in the status field of an executable subsample to open the context menu and select ▶+ **Add to running sample series**.

3 Adding all executable subsamples to an ongoing determination

- Click on ≡+ to add all executable subsamples to the ongoing determination.

The determination of the executable subsamples is executed according to their position in the sample list.

The icon appears below the sample list to the right of ↓ or ↓↓ after a determination has been started.

Planning determinations of subsamples

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Opening the planner

- Click on the subsample status whose determination is to be planned.
- Click in the status field to open the context menu and select to open the planner.

The subsample must be in **Ready** status so that its determination can be planned.

2 Selecting the time of a determination

- In the planner, select the date, hour and minute when the determination of the subsample is to be executed.

3 Selecting the determination type

- Selecting the determination type of the subsample:
  - **Series determination**: The determinations of the subsamples in the list are analyzed sequentially.
  - **Parallel determination:** The determinations of the subsamples in the list are analyzed in parallel.

4 Finishing planning

- Click on **Start planning** to start the determination of the subsample at a defined time.

If determinations in the sample list are already being executed at the planned time, then the subsample will be added to the ongoing sample series.

See also

Displaying live data and controlling the run (chapter 5.10.10, page 316)

Editing sample list (chapter 5.10.1.2, page 212)

Parallel determination – Run (chapter 5.10.8.4, page 299)

Recording samples (chapter 5.10.4.1, page 251)

Recording subsamples (chapter 5.10.7.1, page 273)

Series determination – Run (chapter 5.10.8.3, page 298)

Single determination – Run (chapter 5.10.8.2, page 297)

Stopping a determination (chapter 5.10.8.7, page 308)

Subsamples – Statuses (chapter 5.10.7.3, page 276)

5.10.8.7 Stopping a determination

The determination of a subsample is usually completed automatically. If necessary, the determination can also be stopped manually at any time.

Single determination

1 Stopping a determination

- Click on below the sample list.

The single determination is stopped. The canceled determination now has the status **Canceled after stop**.

Series determination or parallel determination

1 Stopping a determination

- Click on below the sample list.

All currently ongoing determinations are stopped. The canceled determinations now have the status **Canceled after stop**.

The subsamples that have not yet been analyzed once again return to the status **Ready**.

2 Stopping a determination after a delay

- Click on below the sample list.

The running determination is run to its end, but no new determination is started. The executed determinations have the status **Completed**.

The subsamples that have not yet been analyzed once again return to the status **Ready**.

See also

Starting determination (chapter 5.10.8.6, page 304)

Subsamples – Statuses (chapter 5.10.7.3, page 276)

5.10.8.8 Pausing determination

The **Hold determination** function is used to pause the running operating procedure.

Some commands cannot be paused immediately. These commands are executed to the end after clicking on the **Hold determination** function. It is only afterwards that the run is paused. The **Hold after command end** status is displayed in the **Live data** subsection.

Prerequisite:

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Pausing sequence

- In the sample list, click on the status of the subsample to call up the context menu and select **Hold determination**.

A held command is indicated with the status . The **Command on hold** status appears in the **Live data** subsection.

2 Resuming or canceling the run

- In the context menu, click on **Continue** to continue the run or click on **Stop determination** to cancel it.

Commands that can be held

The following commands can be paused:

- Titration commands
- Measuring commands and calibration commands for titration
- Dosing commands, such as **ADD**, **PISTON END** or **FILL**
- Time-controlled commands: **PUMP**, **STIR**, **WAIT** or **READ**
- Additional commands: **REQUEST**

For dosing commands, the execution is paused when the Hold determination function is selected. Clicking on **Continue** causes the command to be resumed at the position where it was paused.
For time-controlled commands, the time sequence is interrupted when the **Hold determination** function is triggered. Clicking on **Continue determination** causes the set time to run to the end.

Commands that cannot be held

The following commands cannot be held:

- Automation commands, e.g. **LIFT**, **OPEN GRIPPER** or **CLOSE GRIPPER**
- All spectroscopy commands, e.g. **MEAS SPEC**, **MEAS REF SPEC**, **PREP SPEC** or **VESSEL REMOVAL**, including the specific commands for calibration and validation and tests, e.g. **CAL WL**, **VAL REF STD** or **TEST NOISE**
- Additional commands, e.g. **WRITE**, **TARE** or **WEIGH**

See also

COND CHECK – Parameters (chapter 5.11.8.15, page 606)

KFT – Properties (chapter 5.11.8.10.1, page 568)

Subsamples – Statuses (chapter 5.10.7.3, page 276)

5.10.8.9 Preparing determination

The instructions summarize all the steps necessary for performing determinations in the OMNIS Software. Links to specific topics are included for additional information on individual steps.

Preparing sample

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Reserving an instrument and creating a work system

- Reserve the desired instruments in **Equipment** ▶ **Instruments**. *(see "Reserving and releasing instruments", chapter 5.12.2.4, page 861)*
- In **Equipment** ▶ **Work systems**, click on + to create a new work system. *(see "Creating a work system", chapter 5.12.4.4, page 989)*

- In the new work system, click on to open the **Inventory** window.
- Use drag and drop to insert the reserved instrument into the work system.
- If necessary, reserve additional instruments and insert them into the work system.
- Save the work system by clicking on .

2 Creating method

- In **Processes** ▶ **Methods**, click on to create a new method. *(see "Creating and editing a method", chapter 5.11.3.3, page 418)*
- In the new method, click on to open the **Properties** window.
- In **Properties** ▶ **Execute with**, select the work system created.

3 Entering and parameterizing commands

- Click on to open the **Library** window and search for the desired commands.
- Use drag-and-drop to insert and parameterize each command individually into the method.
- Select the functional unit required for the command in **Properties** ▶ **Execute with**. *(see "Assigning a functional unit to a command", chapter 5.12.3.3, page 905)*
- If required, insert an optional run. *(see "Creating and editing a method", chapter 5.11.3.3, page 418)*
- Save the method by clicking on .

4 Creating operating procedure

- In **Processes** ▶ **Operating procedure**, click on to create a new operating procedure. *(see "Creating and editing an operating procedure", chapter 5.11.1.3, page 387)*
- Click on to open the **Library** window and use drag and drop in **Library** ▶ **Methods** to insert the method created into the operating procedure.
- If required, insert additional methods into the operating procedure.
- Click on to save the operating procedure.

5 Creating sample profile

- Create a new sample profile under **Samples** ▶ **Sample profiles** by clicking on . *(see "Creating and editing sample profile", chapter 5.10.5.2, page 261)*
- Assign a unique name for the sample profile in the **Name of the sample profile** field. This name is needed to identify the sample profile (see **step 6**) when creating the sample.
- Optionally enter a unique designation for the sample profile in the **Sample profile ID** field. This ID is required when creating the sample based on a **Sample profile ID** (see **step** 6).
- Select the operating procedure created and define the required number of subsamples.
- Save the sample profile by clicking on .

6 Creating and editing sample list

- Under **Samples** ▶ **Sample lists**, click on to create a new sample list. *(see "Creating and deleting sample lists", chapter 5.10.1.1, page 211)*
- In the sample list, select the sample profile created from the selection list and add the required number of samples to the sample list by clicking on .
  or
- Click on to open the **Add samples based on the sample profile IDs** dialog and enter a Sample profile ID. Click on **[Add]** or **[ENTER]** to add the samples contained in the entered sample profile to the sample list.
- Save the sample list by clicking on .

The samples and subsamples are added to the sample list automatically in accordance with the sample profile. If a sample profile has been added using the selection list, then the last selected sample profile remains pre-selected in the input field of the selection list.

7 Carrying out determination

- **Optional**: To process all samples one after the other, select ↓ in the selection list to set the determination as a series determination. To process all samples simultaneously, select ↓↓ in the selection list to set the determination as a parallel determination. The determination as series determination is the default setting.

- Start the determination for all selected subsamples by clicking on . Start the determination for all executable subsamples in the sample list by clicking on . *(see "Starting determination", chapter 5.10.8.6, page 304)*

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Creating a work system (chapter 5.12.4.4, page 989)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Recording samples (chapter 5.10.4.1, page 251)

Reserving and releasing instruments (chapter 5.12.2.4, page 861)

Sample list – Tab (chapter 5.2.2, page 159)

Starting determination (chapter 5.10.8.6, page 304)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.8.10 Determination – Preparation and follow-up

Certain runs are only to be executed once on a work system in a determination series. This allows for the work system to be set to a desired initial state in the beginning or left in a desired final state at the end.

The necessary runs are added in the desired place in the operating procedure with an **IF** command. Variables specific to the work system are used as a condition for the execution. This allows methods with dynamic work system assignment to be used.

A determination series can run as a series determination, a parallel determination and/or across several sample lists.

Variables for the first and last use of the work system

2 variables are available for the scan to determine whether the work system was used for the first or last time. They can be found in the **Assigned work systems** subcategory of the **Equipment variables** variable category.

- '**FirstUse.CurrentWorkSystem**.*Method name*'
  - Variable value = **1**
    The current work system of the method selected in the variable name is used in the determination series for the first time.
  - Variable value = **0**
    The current work system of the method selected in the variable name is **not** used in the determination series for the first time.
- '**LastUse.CurrentWorkSystem**.*Method name*'
  - Variable value = **1**
    The current work system of the method selected in the variable name is used in the determination series for the last time as planned.
  - Variable value = **0**
    The current work system of the method selected in the variable name is **not** used in the determination series for the last time as planned.

After the follow-up run was executed on a work system, the preparation run is executed again when the same work system is used next.

To ensure that the runs are executed at the right moment, the variables must be scanned continuously for every determination of the determination series. In addition, the variables must be scanned for each individual work system for which a preparation run or follow-up run is to be carried out.

Variable for excluding single determinations

If the runs are only to be executed in a determination series and not in a single determination, an additional variable must be used to scan the determination run. It can be found in the **Subsample data** variable category.

- '**ExecutionMode**.**CurrentSubsample**'
  - Variable value = **0**
    The subsample is processed as a **single determination**.
  - Variable value = **1**
    The subsample is processed as a **series determination**.
  - Variable value = **2**
    The subsample is processed as a **parallel determination**.

Application examples

The following conditions can be defined, for example, for the **IF** command with the variables mentioned. With this, the defined runs are executed in series determinations or parallel determinations across one or more sample lists.

- For preparation runs that are not to be executed in the single determination:
  'FirstUse.CurrentWorkSystem.*Method name*' = 1 AND 'ExecutionMode.CurrentSubsample' <> 0
- For follow-up runs that are not to be executed in the single determination:
  'LastUse.CurrentWorkSystem.*Method name*' = 1 AND 'ExecutionMode.CurrentSubsample' <> 0

The *method name* must correspond to a method that was executed on the work system for which a preparation or follow-up run is to be carried out. To avoid errors, the variable should be selected directly from the variable list.

The variables must be inserted again in the formula editor if a method is renamed for which variables are used in the **IF** command.

Further examples for the application in operating procedures are available in the Metrohm Knowledge Base: *Operating procedure – Templates for titration* / *Operating procedures/methods – Templates for TitrIC flex*

See also

IF – Parameters (chapter 5.11.8.70, page 782)

Variables – Directory (chapter 5.11.9.3, page 827)

Work system – Definition (chapter 5.12.4, page 987)

5.10.9 Displaying measuring point list

Prerequisite:

- The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.
  or
- The **Samples** ▶ **Search queries** subsection is opened. A search query is opened and at the front.

1 Selecting subsample

- Select the subsample for which the measuring point list is to be displayed.

2 Displaying measuring point list

- In **Curves and data** ▶ **Measuring point lists**, display the measuring points that were recorded during the determination for the selected subsample.

If there are multiple commands, the measuring point list for the corresponding command can be selected in the selection list . The arrows to the right and left of the selection list are used to switch between the commands.

See also

Copying table (chapter 5.2.8, page 172)

Sample list – Tab (chapter 5.2.2, page 159)

5.10.10 Displaying live data and controlling the run

The live data of the determination is displayed for the subsample selected in the sample list under **Samples** ▶ **Sample list** ▶ **Curves and data** ▶ **Live data**. Here you can follow the progress of the determination. You can switch between simultaneously running determinations and intervene in the determination if necessary. If measured data is generated, it is displayed as a curve and also shown in the measured value window in real time.

Displaying the live data

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.
  or
- The **Samples** ▶ **Search queries** subsection is opened. A search query is opened and at the front.
- The desired subsample is currently running.

1 Selecting a subsample

- Select the subsample for which the live data is to be shown.

2 Displaying the live data

- In **Curves and data** ▶ **Live data**, display the live data that was recorded during the determination for the selected subsample.

If there are multiple commands, the live data for the corresponding command can be selected in the selection list . The arrows to the right and left of the selection list are used to switch between the commands.

During the run of the **COND CHECK** command, the conditioning status (**Conditioning OK** or **Conditioning not OK**) and the stability of the drift are displayed in addition to various current measured values.

Icon	Meaning
	The drift decreases.
	The drift increases.
	The drift is stable.

If the live data of a subsample is accessed after a determination has finished, the last status of the subsample is displayed.

Skipping a command

The **[Skip]** button is shown in the live data while a command is running.

1 Skipping the command

- The running command can be ended prematurely by clicking on **[Skip]**.

Commands that have no actual runtime or that control movements of a sample robot or sample changer cannot be skipped. In this case, the button is not displayed.

The determination is continued with the next command.

Waiting for user input and continuing the determination

If a user action is required (e.g. by the **REQUEST** or **WAIT** command) during the determination, the associated message is shown in the **Live data** subsection.

1 Continuing the determination

- **WAIT** command:
  Click on **[Continue]** to end the waiting time and continue with the run.

- **REQUEST** command:
  - Enter the necessary data.
  - Click on **[Continue]** to confirm the entry and continue with the run.

The determination is continued with the following command.

Ending conditioning prematurely and starting titration

A conditioning command is currently running. The determination is to be started before the **Conditioning OK** status is reached.

1 Starting the titration

- Click on **[Start titration]** during conditioning.

A message is displayed that shows that the system is not conditioned.

2 Starting the titration immediately or continuing with conditioning

- Click on **[Start titration]** again to start the titration anyway.

The titration is started from the **Conditioning not OK** status.

- Click on **[Continue conditioning]** to return to conditioning.

See also

Displaying curves and adjusting the curve display (chapter 5.10.11.1, page 320)

Sample list – Tab (chapter 5.2.2, page 159)

5.10.11 Curves – Properties

Clicking on in **Samples** ▶ **Sample lists** ▶ **Curves and data** ▶ **Curves** opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 3 subsections **Chart – x-axis**, **Chart – y-axis** and **Chart – y2-axis**:

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis. The selection depends on the command type (see command parameters).

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis. The selection depends on the command type (see command parameters).
Displaying regression lines	Display of at least one regression line that runs through the values of the selected quantity. The check box is used for activation. The check box is displayed only if a command of the **MET pH**, **MET COND**, **DET Ipol**, **DET pH** or **DET U** type was used. The regression lines are displayed only if the quantity **Conductivity κ** or **Gran function value** is selected for the corresponding y-axis or y2-axis and the quantity **Volume** is selected for the x-axis. The display is disabled by default. In addition, the measuring points or Gran function values used for the calculation of the regression lines are highlighted. For a Gran evaluation, the volume of the Gran point is also shown as a vertical line. **Note**: Depending on the command, 1 or 2 regression lines are displayed.

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis. The selection depends on the command type (see command parameters).
Displaying regression lines	Display of at least one regression line that runs through the values of the selected quantity. The check box is used for activation. The check box is displayed only if a command of the **MET pH**, **MET COND**, **DET Ipol**, **DET pH** or **DET U** type was used. The regression lines are displayed only if the quantity **Conductivity κ** or **Gran function value** is selected for the corresponding y-axis or y2-axis and the quantity **Volume** is selected for the x-axis. The display is disabled by default. In addition, the measuring points or Gran function values used for the calculation of the regression lines are highlighted. For a Gran evaluation, the volume of the Gran point is also shown as a vertical line. **Note**: Depending on the command, 1 or 2 regression lines are displayed.

See also

Displaying curves and adjusting the curve display (chapter 5.10.11.1, page 320)

Overlaying curves (chapter 5.10.11.6, page 332)

Reevaluating curves (chapter 5.10.11.7, page 335)

5.10.11.1 Displaying curves and adjusting the curve display

These instructions describe functions related to the display of curves, charts and tables in the work areas **Samples** and **Models**.

Requirement for all instructions:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

Displaying curve

Prerequisite:

- The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.
  or
- The **Samples** ▶ **Search queries** subsection is opened. A search query is opened and at the front.

1 Selecting a subsample

- Select the subsample for which the curve is to be displayed.

2 Displaying curves

- Display the recorded measured values as a curve under **Curves and data** ▶ **Live data** while a determination is running.
  or
- Display the recorded measured values as a curve under **Curves and data** ▶ **Curves** while a determination is running or after it has finished.
  or
- Display the curve that was created when calibrating the sensor or executing the standard addition under **Curves and data** ▶ **Calibration curves** while a determination is running or after it has finished.

If there are multiple commands, the curve for the corresponding command can be selected in the selection list . The arrows to the right and left of the selection list are used to switch between the commands.

For calibration curves, you can change between the sensors with the arrows if several sensors are used.

A **green curve** with the quantity selected for the y-axis is displayed by default under **Curves and data** ▶ **Curves**. Optionally, you can define under **Curves and data** ▶ **Curves** ▶ **Properties** that a second **orange curve** with the quantity selected for the y2-axis is also displayed. Additional information for the **Properties** window: *(see "Curves – Properties", chapter 5.10.11, page 318)*

Hiding and showing the measured value window or details window

Prerequisite:

- The **Samples** ▶ **Sample lists** or **Samples** ▶ **Search queries** subsection is opened.
- The **Live data** area is visible.

  or
- The **Models** ▶ **Quantification models** or **Models** ▶ **Slope/y-intercept corrections** subsection is opened.
- One of the following areas is visible:
  - **Correlation plot**
  - **Figures of merit**

1 Hiding the measured value window or details window

- Right-click in the chart.
- Select **[Show/hide measured value window]** in the context menu.

  or
- Select **[Show/hide details window]** in the context menu.

The measured value window or details window is hidden.

2 Showing the measured value window or details window

- Right-click in the chart.
- Select **[Show/hide measured value window]** in the context menu.

  or
- Select **[Show/hide details window]** in the context menu.

The measured value window or details window is shown.

Functions for all charts

The following instructions apply for all charts in the **Samples** and **Models** work areas.

1 Copying chart

- Right-click in the chart.
- Select **[Copy chart]** in the context menu.

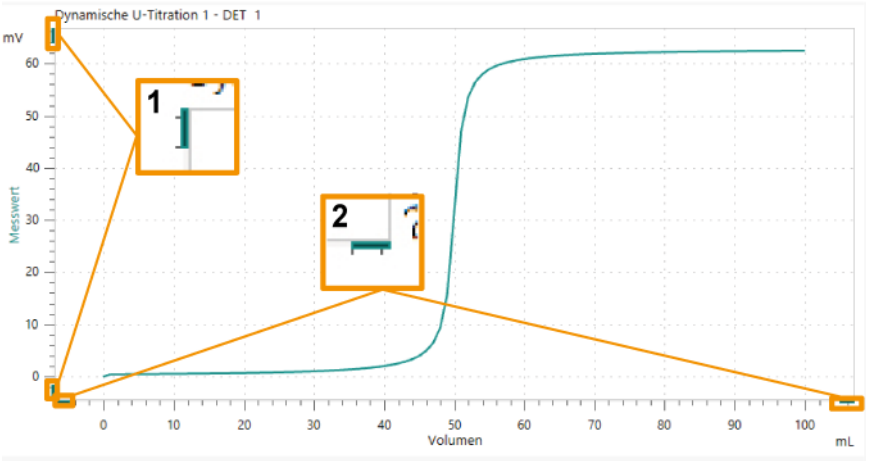
The chart is copied to the clipboard.

If the chart has a table, then this can also be copied. Additional information on copying tables: *(see "Copying table", chapter 5.2.8, page 172)*

2 Inserting chart

- Open the required file in which the chart is to be inserted.
- Insert the chart into the file.

Scaling axes



1 Zooming in the chart

- Position the cursor on the left of the desired area.
- With the left mouse button held down, drag a rectangle over an area from left to right.

The desired area is magnified.

2 Zooming chart vertically

- Position the cursor on the zooming element **(1)** until the cursor is displayed as ⇳.
- Move along the y-axis with the left mouse button pressed down.
  - Move up: Increase area vertically.
  - Move down: Decrease area vertically.

3 Zooming chart horizontally

- Position the cursor on the zooming element **(2)** until the cursor is displayed as ⇔.
- Move along the x-axis with the left mouse button pressed down.
  - Move to the right: Increase area horizontally.
  - Move to the left: Decrease area horizontally.

Scaling axes with keyboard and cursor

1 Positioning cursor

- Position the cursor on the desired section in the chart.

2 Zooming chart vertically

- Rotate the mouse wheel while holding the **[CTRL]** key pressed down.
  - Rotate forward: Increase section vertically.
  - Rotate backward: Decrease section vertically.

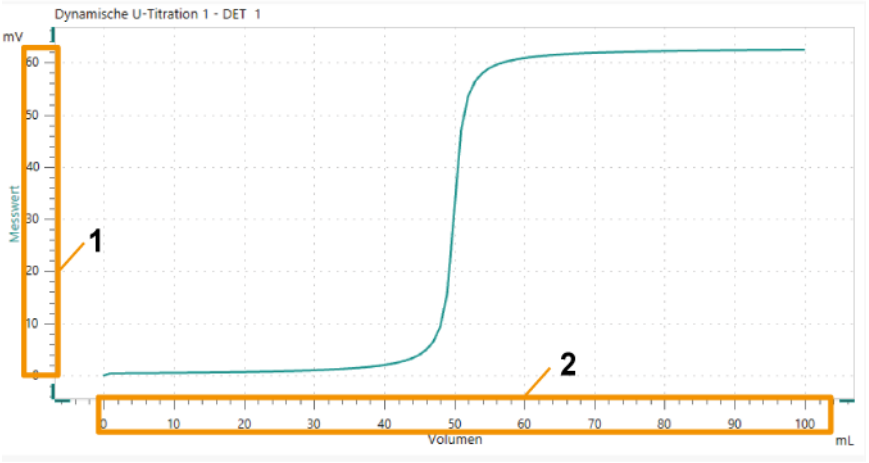
3 Zooming chart horizontally

- Rotate the mouse wheel while holding the **[SHIFT]** key pressed down.
  - Rotate forward: Increase section horizontally.
  - Rotate backward: Decrease section horizontally.

4 Scaling x-axis and y-axis together

- Rotate the mouse wheel.
  - Rotate forward: Increase section horizontally and vertically.
  - Rotate backward: Reduce size of section horizontally and vertically.

Moving displayed area



1 Moving displayed area vertically

- Position the cursor on the number area of the y-axis **(1)**.
- Move the curve by rotating the mouse wheel:
  - Rotate forward: Moves to lower value range.
  - Rotate backward: Moves to higher value range.
- Move the curve by holding down the left mouse button.
  - Move upward: Moves to lower value range.
  - Move downward: Moves to higher value range.

2 Moving the displayed area horizontally

- Position the cursor on the number area of the x-axis **(2)**.
- Move the curve by rotating the mouse wheel:
  - Rotate forward: Moves to lower value range.
  - Rotate backward: Moves to higher value range.
- Move the curve by holding down the left mouse button.
  - Move to the right: Moves to lower value range.
  - Move to the left: Moves to higher value range

3 Moving displayed area

- Position the cursor on the desired curve section.
- Move the curve in the desired direction by holding the right mouse button pressed down.

Resetting display

1 Resetting display

- Right-click in the chart.
- Select **Reset view** in the context menu.
- Alternatively, with the left mouse button held down, drag a rectangle over an area from right to left.

The chart is reset to the default view.

See also

Curves – Properties (chapter 5.10.11, page 318)

Displaying live data and controlling the run (chapter 5.10.10, page 316)

Displaying measuring point list (chapter 5.10.9, page 315)

Reevaluating curves (chapter 5.10.11.7, page 335)

5.10.11.2 Curves – Window-based evaluation

The window definitions can be individually added by clicking on or deleted by clicking on .

The areas of the individual evaluation windows must not overlap. The lower limit must always be smaller than the upper limit.

If the window type is changed retrospectively, all window definitions are reset.

Potentiometric evaluation and Conductometric evaluation

The Potentiometric evaluation and the Conductometric evaluation can be carried out with or without window evaluation.

For the evaluation with window evaluation, equivalence points are only recognized if they lie within the evaluation window and if they meet the parameters defined for the respective window. A maximum of 1 EP per evaluation window can be recognized.

A maximum of 9 evaluation windows can be defined when the window evaluation is activated. You can choose between Volume window and Measured value window (depending on the selected quantity - pH window, Potential window, Potential window or Conductivity window).

The following parameters can be defined for each evaluation window:

Definitions for the window evaluation	
Lower limit	Defines the lower limit of the evaluation window. The lower limit is part of the evaluation window.

Definitions for the window evaluation	
Upper limit	Defines the upper limit of the evaluation window. The upper limit is not part of the evaluation window.
EP criterion	Threshold value for the evaluation of equivalence points. Equivalence points are not evaluated if the calculated ERC value (ERC = Equivalence point Recognition Criterion) is smaller than the defined EP criterion.
EP recognition	Filters for the recognition of equivalence points: ▪ **First** Of the evaluated equivalence points, only the first is recognized. ▪ **Last** Of the evaluated equivalence points, only the last is recognized. ▪ **Greatest** Of the evaluated equivalence points, only the one with the greatest ERC value (i.e. with the steepest curve section) is recognized.

Break point evaluation

The Break point evaluation can be carried out with or without window evaluation.

For the Break point evaluation with window evaluation, break points (BPs) are only recognized if they lie within the evaluation window and if they meet the parameters defined for the respective window. A maximum of 1 BP per evaluation window can be recognized.

A maximum of 9 evaluation windows can be defined when the window evaluation is activated. You can choose between Volume window and Measured value window (depending on the selected quantity - pH window or Potential window).

The following parameters can be defined for each evaluation window:

Break point evaluation	
Lower limit	Defines the lower limit of the evaluation window. The lower limit is part of the evaluation window.
Upper limit	Defines the upper limit of the evaluation window. The upper limit is not part of the evaluation window.
BP criterion	Criterion for the evaluation of break points. Standardized difference between maximum and minimum of the second derivative. Break points with a smaller BRC value than the value entered here will not be evaluated.
Min. deflection	Threshold value of the slope difference between the sections before and after the break point. The smaller the difference, the more break points will be found.

Break point evaluation	
Max. expected BPs	Maximum number of break points that are expected. The curve is smoothed until the number of evaluated break points is smaller or equal to this number.
BP recognition	Filters for the recognition of break points: ▪ **First** Of the evaluated break points, only the first is recognized. ▪ **Last** Of the evaluated break points, only the last one is recognized.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Lower limit**
  Minimum value Potential window and Potential window: –1,200.0 mV
  Maximum value Potential window and Potential window: 1,200.0 mV
  Minimum value pH window: –13.000
  Maximum value pH window: 20.000
- **Upper limit**
  Minimum value Potential window and Potential window: –1,200.0 mV
  Maximum value Potential window and Potential window: 1,200.0 mV
  Minimum value pH window: –13.000
  Maximum value pH window: 20.000

See also

Curves – Automatic evaluation (chapter 5.10.11.7.1, page 336)

Curves – Manual evaluation (chapter 5.10.11.7.2, page 342)

DET – Properties (chapter 5.11.8.3.1, page 445)

MET – Properties (chapter 5.11.8.4.1, page 472)

Reevaluating curves (chapter 5.10.11.7, page 335)

5.10.11.3 Curves – Fixed point evaluation

With the fixed point evaluation, fixed points can be determined with the data from the measuring point list and they can then be used to calculate results, for example. A fixed point can be defined using one of the following 3 measured quantities:

- Measured value (conductivity κ, pH value, potential, voltage or temperature)
- Volume or water
- Time

The values of the other two measured quantities are calculated and are available as variables.

By clicking , a new measured value can be defined as a fixed point. A fixed point can be deleted again with . Up to 9 fixed points can be defined.

The following parameters can be defined for each fixed point:

Definitions for the fixed points	
Specified quantity	Selection of the specified quantity for the calculation of the fixed point from the measuring point list.
Fixed point at	Specified measured value for the calculation of the fixed point.

See also

DET – Properties (chapter 5.11.8.3.1, page 445)

KFT – Properties (chapter 5.11.8.10.1, page 568)

MET – Properties (chapter 5.11.8.4.1, page 472)

SET – Properties (chapter 5.11.8.6.1, page 512)

5.10.11.4 Curves – Gran evaluation

Principle

The evaluation of titrations in accordance with the Gran procedure takes place through a linearization of the titration curve and is used for the determination of the equivalence point. To accomplish this, the corresponding Gran function value is calculated for each measuring point with the Gran function, and this is applied in the Gran plot against the dosed volume of the titrant. The Gran point is defined by the determination of a regression line in the segment before the equivalence point or in the segment after the equivalence point. If only one segment is used for the evaluation, then the Gran point will correspond to the intersection point of the lines of regression with the x-axis (when Gran function value = 0). If both segments are used, then the intersection point of the two lines of regression corresponds to the Gran point. In contrast to the potentiometric evaluation, for which the measuring points in the jumping range are decisive, in the case of the Gran evaluation it is the measuring points before or after the equivalence point which are evaluated. Titrations with small changes of potential can also be evaluated as a result (e.g. titrations of weak acids with strong bases).

The Gran function used for linearization of the titration curve depends on two factors:

- Reaction type (analyte, titrant)
- Evaluation range of the titration curve (segment before the equivalence point, segment after the equivalence point or both segments)

The Gran function and the linear range used for the calculation of the regression lines can be defined in the Properties of the titration command under **Gran evaluation** by selecting the reaction type and the segment to be used. During the titration, the Gran function value *G* is calculated from the dosed volume of the titrant *V(t)*, from the measured value (e.g. pH value *pH(t)*) and, depending on the reaction type and segment, from the initial volume V_0 and added to the measuring point list for each measuring point. The Gran function value on each axis can be selected as a quantity and as a result displayed as a curve in the curve display under **Curves and data** ▶ **Curves**. In accordance with the principle of the least squares method, a regression line is placed through the Gran function values in the part of the segment that is defined in the titration command by the lower limit and the upper limit. The regression line is displayed only in the Gran plot, i.e. if the quantity **Gran function value** is selected for the y-axis and the quantity **Volume** is selected for the x-axis. The Gran point determined by the evaluation is displayed in the titration curve.

The following Gran functions are used for acid-base titrations in accordance with Gunnar Gran (1952. Determination of the Equivalence Point in Potentiometric Titrations. Part II. The Analyst, 77, 661-671):

Reaction type	Segment	Gran function	Scaling factor *k*
Weak monoprotic acid, strong base	Acidic segment before the equivalence point	$G_{before}(V(t), pH(t)) = V(t) \cdot 10^{(k - pH(t))}$	0
	Alkaline segment after the equivalence point	$G_{after}(V(t), pH(t)) = (V_0 + V(t)) \cdot 10^{(pH(t) - k)}$	10
Weak monoprotic base, strong acid	Alkaline segment before the equivalence point	$G_{before}(V(t), pH(t)) = V(t) \cdot 10^{(pH(t) - k)}$	10
	Acidic segment after the equivalence point	$G_{after}(V(t), pH(t)) = (V_0 + V(t)) \cdot 10^{(k - pH(t))}$	0
Strong acid, strong base	Acidic segment before the equivalence point	$G_{before}(V(t), pH(t)) = (V_0 + V(t)) \cdot 10^{(k - pH(t))}$	0
	Alkaline segment after the equivalence point	$G_{after}(V(t), pH(t)) = (V_0 + V(t)) \cdot 10^{(pH(t) - k)}$	10
Strong base, strong acid	Alkaline segment before the equivalence point	$G_{before}(V(t), pH(t)) = (V_0 + V(t)) \cdot 10^{(pH(t) - k)}$	10
	Acidic segment after the equivalence point	$G_{after}(V(t), pH(t)) = (V_0 + V(t)) \cdot 10^{(k - pH(t))}$	0

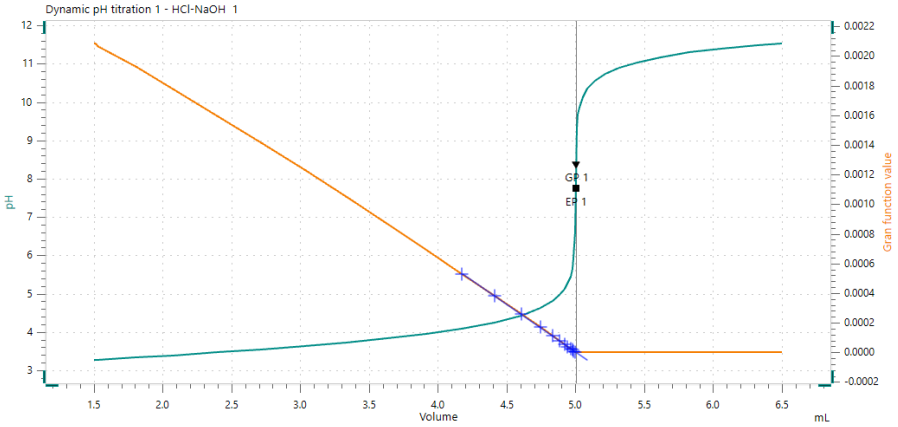
The scale factor *k* depends on the selection of the reaction type and of the segment and is used for scaling the Gran function values. The scale factor has no influence on the position of the Gran point in the Gran plot.

Example of a Gran evaluation in 1 segment

Reaction type	Strong acid, strong base
Gran plot	Acidic segment

The following elements are shown in the curve display:

- Gran plot consisting of the Gran function values
- Regression line
- Markings (+) of the Gran function values used for the regression line
- Gran point (GP) and volume of the Gran point as a vertical line

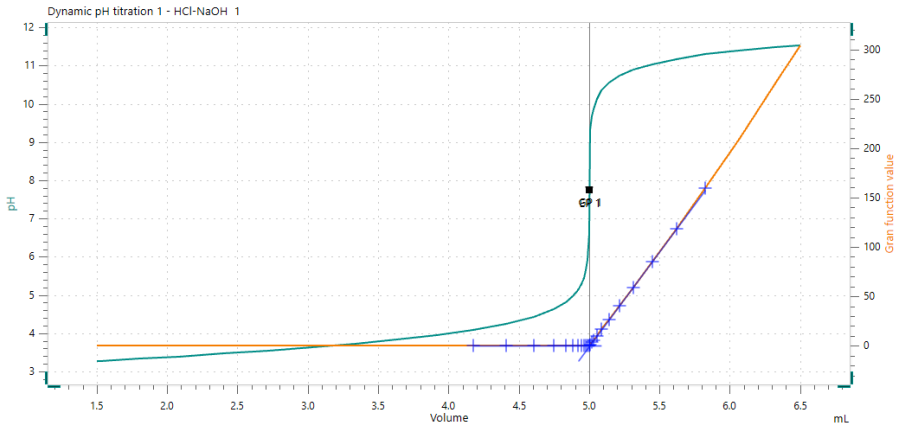


Example of a Gran evaluation in 2 segments

Reaction type	Strong acid, strong base
Gran plot	Acidic and alkaline segment

The following elements are shown in the curve display:

- Gran plot consisting of the Gran function values
- Regression lines
- Markings (+) of the Gran function values used for the regression line
- Gran point (GP) and volume of the Gran point as a vertical line



See also

DET – Properties (chapter 5.11.8.3.1, page 445)

DET – Run (chapter 5.11.8.3.2, page 463)

MET – Properties (chapter 5.11.8.4.1, page 472)

MET – Run (chapter 5.11.8.4.2, page 491)

5.10.11.5 Curves – Thermometric evaluation

With the thermometric evaluation, the ERC curve can be evaluated automatically and possible equivalence points can be recognized by defined EP conditions. For each equivalence point to be recognized, an EP condition consisting of reaction type and EP criterion is defined.

Further information on the thermometric evaluation: *(see "TET – Principle", chapter 5.11.8.5, page 497)*

By clicking on , a new condition for an equivalence point can be defined. can be used to delete the EP condition once again. Up to 9 EP conditions can be defined.

The following parameters can be defined for each equivalence point:

Definitions for the EP conditions	
Reaction type	Reaction type for the evaluation of the titration curve. ▪ **Endothermic**: The ERC value of the equivalence point is positive. ▪ **Exothermic**: The ERC value of the equivalence point is negative.
EP criterion	Threshold value for the evaluation of equivalence points. Equivalence points are not recognized if the absolute value of the ERC value (ERC = **E**quivalence point **R**ecognition **C**riterion) is smaller than the absolute amount of the defined threshold value.

See also

TET – Principle (chapter 5.11.8.5, page 497)

TET – Properties (chapter 5.11.8.5.1, page 501)

5.10.11.6 Overlaying curves

Curves of different subsamples can be shown together in one curve display. For this, at least one subsample must be selected. The selected subsamples can be part of different samples of a sample list.

1 Selecting a subsample

- In **Samples** ▶ **Sample lists**, select the desired sample list.
- Double-click on the entry in the overview list to open the sample list.
- Select one or more subsamples from the sample list to display the desired curves.

Additional information about selecting several subsamples: *(see "Editing sample list", chapter 5.10.1.2, page 212)*

2 Displaying curves

- Activate the curve overlay by clicking on under **Curves and data** ▶ **Curves**.

The curves of the selected subsamples are displayed with the previously used curve properties.

Additional subsamples can be selected if necessary to add their curves to the curve overlay.
The values for the x-axis and y-axis are taken from the first subsample selected for the curve overlay.

If the icon is not displayed, then the area must be enlarged by dragging the divider.

Actions in the overview list and in the chart

1 Sorting curves

- Sort the displayed curves by clicking on the required column header in the overview list.

2 Selecting and highlighting curves

- Clicking on a curve in the chart or in the overview list causes these to be highlighted in the chart and in the overview list.

- Once a curve is selected, additional curves can be added to the selection and highlighted by clicking while holding down the **[CTRL]** key.
- In the overview list, all curves in between can furthermore be added to the selection by clicking on another curve while holding down the **[SHIFT]** key. If multiple objects are already selected, then clicking on a different curve with the key combination **[CTRL]**+**[SHIFT]** causes all of the curves in between to be added to the selection.

Click with the **[CTRL]** key pressed down to deselect a curve once again after it has been selected.

3 Hiding and showing curves

- Hide a curve by deactivating the check box in the first column of the overview list.
  or
- Select one or more curves in the overview list and right-click to open the context menu. Click on **[Hide]** to hide the curves.

Enable the check box or click on **[Show]** in the context menu to show the curves again.

Displaying curves with offset

1 Enabling curve offset

- Click on to open the **Properties** window.
- Enable the **Apply curve offset** check box to display the curves starting from a defined point on the reference curve with an offset. By default, the first curve displayed in the overview list is set as the reference curve. The reference curve is displayed in bold in the overview list.
  Note: Once the curve offset is applied, the values on the axes are correct only for the reference curve.

2 Defining the reference point and offset

- Enter the X value for the reference point and the offset for the x axis and the y axis: *(see "Curve overlay – Properties", chapter 5.10.11.6.1, page 334)*

3 Changing the reference curve (optional)

- In the overview list of curves, select the curve to be used as the new reference for the curve offset.

- Right-click to open the context menu and select **[Set as reference curve]**.

See also

Curve overlay – Properties (chapter 5.10.11.6.1, page 334)

Curves – Properties (chapter 5.10.11, page 318)

Displaying curves and adjusting the curve display (chapter 5.10.11.1, page 320)

Reevaluating curves (chapter 5.10.11.7, page 335)

5.10.11.6.1 Curve overlay – Properties

Clicking under **Samples** ▶ **Sample lists** ▶ **Curves and data** ▶ **Curves** ▶ **Curve overlay** opens the **Properties** window. The following functions and information are available in the **Curve offset** subsection:

Curve offset	
Apply curve offset	Display of curves with an offset starting from a defined point on the reference curve. By default, the first curve displayed in the overview list is set as the reference curve. The reference curve is displayed in bold in the overview list. The check box is used to enable the curve offset. The curve offset is disabled by default. If the check box is enabled, then the following specific parameters are displayed: ▪ **Reference point (x-value)** ▪ **Offset x-axis** ▪ **Offset y-axis** **Note**: Once the curve offset is applied, the values on the axes are correct only for the reference curve.
Reference point (x-value)	Enter X-value of the point on the reference curve from which the offset originates. If no offset is set, then all curves are overlaid at this point. The unit of the entered value corresponds to the unit on the x axis.
Offset x-axis	Enter offset on the x axis. The curves are offset horizontally by the entered percentage value of the length of the reference curve.
Offset y-axis	Enter offset on the y axis. The curves are offset vertically by the entered percentage value of the height of the reference curve.

The reference curve can be changed in the overview list of curves via the context menu. Additional information on overlaying curves: *(see "Overlaying curves", chapter 5.10.11.6, page 332)*

See also

Displaying curves and adjusting the curve display (chapter 5.10.11.1, page 320)

Overlaying curves (chapter 5.10.11.6, page 332)

5.10.11.7 Reevaluating curves

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
  The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.

1 Selecting a subsample

- Select the subsample for which the curve is to be displayed.

2 Displaying the curve

- Display the recorded measured values as a curve under **Curves and data** ▶ **Curves**.

If there are multiple commands, the curve for the corresponding command can be selected in the selection list . The arrows to the right and left of the selection list are used to switch between the commands.

3 Opening the window Reevaluation

- Click on to open the **Reevaluation** window.

4 Changing the evaluation mode for reevaluation (equivalence point titration only)

- Clicking **[Automatic]** makes it possible to change the evaluation parameters of the automatic evaluation.
  or
- Clicking **[Manual]** makes it possible to edit equivalence points manually.

5 Changing the evaluation parameters

- Change the evaluation parameters as needed for the automatic evaluation mode: *(see "Curves – Automatic evaluation", chapter 5.10.11.7.1, page 336)*
  or
- Add, edit or remove equivalence points for manual evaluation mode: *(see "Curves – Manual evaluation", chapter 5.10.11.7.2, page 342)*

The curve is reevaluated with the modified parameters as soon as the field in which the changes have been made is exited. The recalculated or added points are displayed in the curve and updated in the tables (EP, FP, BP, GP) under **Results** ▶ **Raw data**.

The subsample with the reevaluated curves is marked with .

6 Discarding changes

- If you want to discard the changes, click under **Curves and data** ▶ **Curves** ▶ **Reevaluation**.

The evaluation parameters will be reset to the last saved state.

7 Saving the sample list

- Save the sample list by clicking on .

The subsample with the reevaluated curves is marked with .

See also

Curves – Properties (chapter 5.10.11, page 318)

Displaying curves and adjusting the curve display (chapter 5.10.11.1, page 320)

5.10.11.7.1 Curves – Automatic evaluation

Clicking under **Samples** ▶ **Sample list** ▶ **Subsample** ▶ **Curves and data** ▶ **Curves** opens the **Reevaluation** window. Depending on the titration command, the following functions and parameters are available:

In the case of equivalence point titrations, the functions and parameters for the automatic evaluation mode in the **Reevaluation** window are displayed only if the **[Automatic]** evaluation mode is selected in the window. If equivalence points have been previously added or deleted in the manual evaluation, then these changes will be reset once again with the next automatic evaluation.

Potentiometric evaluation	
Selection of the type	Selection whether the equivalence points are evaluated and recognized throughout the entire titration curve (**Regular**) or only in certain segments of the curve (**Window-based**). The fields **EP criterion** and **EP recognition** only appear in the **Regular** setting. If **Window-based** is selected, then multiple evaluation windows can be defined or edited: *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*.
EP criterion	Threshold value for the evaluation of equivalence points. Equivalence points are not evaluated if the calculated **ERC** value (ERC = **E**quivalence point **R**ecognition **C**riterion) is smaller than the defined value.
EP recognition	Filters for the recognition of equivalence points: ▪ **All** All evaluated equivalence points are recognized. ▪ **Last** Of the evaluated equivalence points, only the last is recognized. ▪ **Greatest** Of the evaluated equivalence points, only the one with the greatest ERC value (i.e. with the steepest curve section) is recognized. ▪ **Off** The evaluation and recognition of equivalence points is switched off.
[Edit evaluation windows]	The window for defining the evaluation windows is opened: *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*

Conductometric evaluation	
Evaluation start	Volume at which the conductometric evaluation is started. The evaluation takes place after the titration. Only measuring points whose volume is greater than or equal to the defined value are taken into account.
Smoothing factor	Factor that determines the smoothing of the titration curve. The higher this value, the more the noise is damped and the titration curve is smoothed. The smoothing of the titration curve has an influence on the ERC curve and the drift and can cause a shift of the equivalence point. The value of the smoothing factor must not be higher than half of the number of measuring points. The maximum value is 25.
Extension of the linear range	Threshold value for the definition of the linear range before and after an ERC extreme point of the ERC curve. The linear range is extended to the point where the ERC value is smaller than the product of the entered percentage value and the ERC of the considered extreme point.

Conductometric evaluation	
Weighting factor	Factor that determines to what extent measuring points in the curved areas of the titration curve are taken into account for the calculation of the regression line. The larger the factor, the less such measuring points are included. 0 means that all measuring points are weighted equally.
Selection of the type	Selection whether the equivalence points are evaluated and recognized throughout the entire titration curve (**Regular**) or only in certain segments of the curve (**Window-based**). The fields **EP criterion** and **EP recognition** only appear in the **Regular** setting. If **Window-based** is selected, then multiple evaluation windows can be defined or edited *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*.
EP criterion	Threshold value for the evaluation of equivalence points. Equivalence points are not evaluated if the calculated **ERC** value (ERC = **E**quivalence point **R**ecognition **C**riterion) is smaller than the defined value.
EP recognition	Filters for the recognition of equivalence points: ▪ **All** All evaluated equivalence points are recognized. ▪ **Last** Of the evaluated equivalence points, only the last is recognized. ▪ **Greatest** Of the evaluated equivalence points, only the one with the largest ERC value (i.e. with the sharpest break) is recognized.
[Edit evaluation windows]	The subsection for defining the evaluation windows is opened. *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*
Thermometric evaluation	
Filtering factor	Factor that determines the smoothing of the titration curve. The higher this value, the more the noise is damped and the titration curve is smoothed. The smoothing of the titration curve by the filtering factor has an influence on the ERC curve and the slope and can cause a shift of the equivalence point. Additional information on the filtering factor: *(see "TET – Principle", chapter 5.11.8.5, page 497)*

Thermometric evaluation	
Damping until	The ERC curve is dampened from the start of the measurement to the defined volume. The start volume is not taken into account at this time. The damping minimizes the influence of titration artifacts (e.g. outliers) that occur at the beginning of the measurement and could be misinterpreted as equivalence points. It is a linear function with a positive slope, i.e. its influence is greatest at the start of the measurement and decreases linearly as the defined volume is reached. The defined volume must be before the first equivalence point. Further information on damping: *(see "TET – Principle", chapter 5.11.8.5, page 497)*
Evaluation start	The thermometric evaluation starts as soon as the defined volume has been dosed since the start of the titration (including start conditions).
Sort equivalence points by	For the recognition of the equivalence points, they are compared with the defined EP conditions according to the selected sorting. ▪ **Volume (ascending)**: The possible equivalence points are sorted by increasing volume. ▪ **Peak height (descending)**: The possible equivalence points are sorted by decreasing peak height. Further information on the thermometric evaluation: *(see "TET – Principle", chapter 5.11.8.5, page 497)*
Define EP conditions	The window for defining the conditions for equivalence points is opened: *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*

Fixed point evaluation	
Specified quantity	Selection of the specified quantity for the calculation of the fixed point from the measuring point list.
Fixed point at	Specified measured value for the calculation of the fixed point.

Break point evaluation	
Selection of the type	Selection whether the break points are evaluated throughout the entire titration curve (**Regular**) or only in certain segments of the curve (**Window-based**) or not at all (**Off**). If **Window-based** is selected, then multiple evaluation windows can be defined or edited: *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*.
BP criterion	Criterion for the evaluation of break points. Standardized difference between maximum and minimum of the second derivative. Break points with a found **BRC** value (BRC = **B**reakpoint **R**ecognition **C**riterion) that is smaller than the value entered here will not be evaluated.

Break point evaluation	
Min. deflection	Threshold value of the slope difference between the sections before and after the break point. The smaller the difference, the more break points will be evaluated.
Max. expected BPs	Maximum number of break points that are expected. The curve is smoothed until the number of evaluated break points is smaller or equal to this number.
BP recognition	Filters for the recognition of break points: ▪ **All** All evaluated break points are recognized. ▪ **First** Of the evaluated break points, only the first one is recognized. ▪ **Last** Of the evaluated break points, only the last one is recognized.
[Edit evaluation windows]	The window for defining the evaluation windows is opened. *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*

Gran evaluation	
Selection of the type	Selection as to whether the titration curve is evaluated according to the Gran procedure (**Gran point**) or not (**Off**). If **Gran point** is selected, then a Gran point is determined for the titration.
Reaction type	Selection of the reaction type (analyte, titrant). The available options for the parameter **Gran plot** are displayed, depending on the selection. ▪ **Weak monoprotic acid, strong base**: Titration of a weak monoprotic acid with a strong base. ▪ **Weak monoprotic base, strong acid**: Titration of a weak monoprotic base with a strong acid. ▪ **Strong base, strong acid or strong acid, strong base**: Titration of a strong base with a strong acid or a strong acid with a strong base.

Gran evaluation	
Gran plot	Range of the titration curve that is used to determine the Gran point. Specifying the lower limit and the upper limit for the selected segment makes it possible to define the linear range in which the measuring points for the determination of the regression line are used. Depending on the selection of the reaction type, the parameters for the Gran function used for the evaluation can also be defined. ▪ **Acidic segment**: If the analyte is acidic, then the segment is used before the equivalence point. If the analyte is alkaline, then the segment after the equivalence point is used. If **Acidic segment** is selected, the following specific parameters appear: – **Initial volume** (does not apply for Weak monoprotic acid, strong base) – **Lower limit pH acidic** – **Upper limit pH acidic** ▪ **Alkaline segment**: If the analyte is acidic, then the segment after the equivalence point is used. If the analyte is alkaline, then the segment before the equivalence point is used. If **Alkaline segment** is selected, the following specific parameters appear: – **Initial volume** (does not apply for Weak monoprotic base, strong acid) – **Lower limit pH alkaline** – **Upper limit pH alkaline** ▪ **Acidic and alkaline segment**: Not only the segment before the equivalence point but also the segment after the equivalence point are both used. If **Acidic and alkaline segment** is selected, the following specific parameters appear: – **Initial volume** – **Lower limit pH acidic** – **Upper limit pH acidic** – **Lower limit pH alkaline** – **Upper limit pH alkaline** **Note:** The **Lower limit pH** and the **Upper limit pH** must be defined for each segment in such a way that both limits are located on the same side of the equivalence point. ▪ **Normalized**: The entire titration curve is used. The standardized procedure is available only for the reaction type **Strong base, strong acid or strong acid, strong base**. If **Normalized** is selected, the following specific parameters appear: – **Initial volume** – **Lower limit pH** – **Upper limit pH** **Note:** The selection **Normalized** corresponds to the evaluation procedure in previous Metrohm applications. Additional information regarding the Gran functions applied: *(see "Curves – Gran evaluation", chapter 5.10.11.4, page 328)*

Gran evaluation	
Initial volume	Volume of the analyte that is in the sample vessel before the titration is started. **Note:** The Gran function values in the measuring point list and the Gran point are recalculated in the event of a change in the initial volume.
Lower limit pH acidic, **Lower limit pH alkaline** or **Lower limit pH**	Defines the lower limit of the range in which the measuring points for determining the regression line are used. **Note:** The Gran point is recalculated in the event of a change in the lower limit when **Acidic segment**, **Alkaline segment** or **Acidic and alkaline segment** is selected. If **Normalized** is selected, then the Gran function values in the measuring point list are recalculated and the Gran plot is rescaled in the event of a change to the lower limit.
Upper limit pH acidic, **Upper limit pH alkaline** or **Upper limit pH**	Defines the upper limit of the range in which the measuring points for determining the regression line are used. **Note:** The Gran point is recalculated in the event of a change in the upper limit when **Acidic segment**, **Alkaline segment** or **Acidic and alkaline segment** is selected. If **Normalized** is selected, then the Gran function values in the measuring point list are recalculated and the Gran plot is rescaled in the event of a change to the upper limit.

See also

Curves – Fixed point evaluation (chapter 5.10.11.3, page 327)

Curves – Gran evaluation (chapter 5.10.11.4, page 328)

Curves – Manual evaluation (chapter 5.10.11.7.2, page 342)

DET – Properties (chapter 5.11.8.3.1, page 445)

MET – Properties (chapter 5.11.8.4.1, page 472)

Reevaluating curves (chapter 5.10.11.7, page 335)

SET – Properties (chapter 5.11.8.6.1, page 512)

5.10.11.7.2 Curves – Manual evaluation

Clicking under **Samples** ▶ **Sample list** ▶ **Subsample** ▶ **Curves and data** ▶ **Curves** opens the **Reevaluation** window. The following functions are available for equivalence point titrations for evaluation mode **[Manual]**:

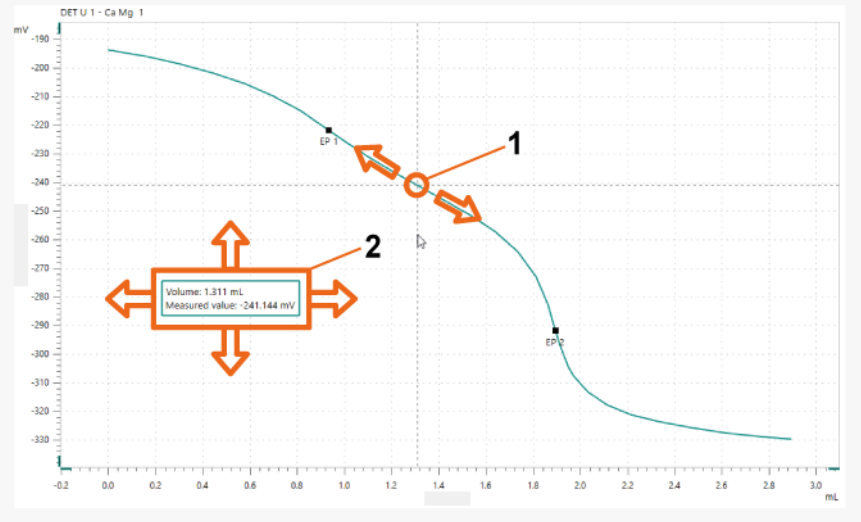
To edit equivalence points (EPs) manually, at least one of the following quantities must be selected for the x-axis or y-axis in the Properties of the curve:

- Volume
- Time

	[Add EP] Click the curve to add an additional equivalence point. The equivalence points are renumbered automatically. A crosshair is displayed as an aid to positioning the equivalence point on the curve (*Positioning the crosshair*).
	[Remove EP] Click an equivalence point to remove that equivalence point. The equivalence points are renumbered automatically.

Positioning the crosshair

The crosshair is used as an aid for positioning the equivalence point on the curve and can be shifted along the volume axis or the time axis by moving the cursor.



A measured value window shows the current curve coordinates of the crosshair position **(1)**. The measured value window **(2)** can be moved by clicking and dragging.

See also

Curves – Automatic evaluation (chapter 5.10.11.7.1, page 336)

Curves – Properties (chapter 5.10.11, page 318)

Displaying curves and adjusting the curve display (chapter 5.10.11.1, page 320)

Reevaluating curves (chapter 5.10.11.7, page 335)

5.10.12 Displaying linear regression

These instructions describe the functions connected with the presentation of the regression lines in the work area **Samples**.

Displaying linear regression

Prerequisite:

- The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.
  or
- The **Samples** ▶ **Search queries** subsection is opened. A search query is opened and at the front.

1 Selecting the sample or subsample

- Select a sample or subsample for which the regression line is to be displayed.
  If a sample is selected, the results for all subsamples of this sample with a statistical correlation will be displayed.
  If a subsample is selected, then only those results will be displayed which were available at the time of the determination of the subsample.

All the subsamples of a sample that were analyzed with the same versions of the operating procedure and of the methods are contiguous for the statistical evaluation.

2 Displaying the regression line

- Display the results of the regression analysis as a line under **Curves and data** ▶ **Linear regression** while a determination is running or after it has finished.

If there are multiple regression commands, the regression line for the corresponding command can be selected in the selection list . The arrows to the right and left of the selection list are used to switch between the commands.
The version of the operating procedure used and the method in abbreviated form are output in the selection list in order to be able to distinguish between the determinations.

A table with information for each subsample that was included in the regression analysis is displayed under the regression lines. Subsamples with invalid values are not displayed in the regression lines, but are listed in the table.

Hiding and showing the measured value window

Prerequisite:

- The **Samples** ▶ **Sample lists** or **Samples** ▶ **Search queries** subsection is opened.
- The **Linear regression** subsection is visible.

1 Hiding the measured value window

- Right-click in the chart.
- Select **[Show/hide measured value window]** in the context menu.

The measured value window is hidden.

2 Showing the measured value window

- Right-click in the chart.
- Select **[Show/hide measured value window]** in the context menu.

The measured value window is shown.

Additional information regarding the functions and presentation options for all charts: *(see "Displaying curves and adjusting the curve display", chapter 5.10.11.1, page 320)*

See also

Displaying curves and adjusting the curve display (chapter 5.10.11.1, page 320)

EVAL LINEAR REGRESSION – Parameters (chapter 5.11.8.68, page 776)

Reprocessing Sample statistics (chapter 5.10.13.2, page 352)

Reprocessing calculations (chapter 5.10.13.1.1, page 350)

Reprocessing linear regression (chapter 5.10.12.1, page 345)

5.10.12.1 Reprocessing linear regression

The results of the linear regression for selected samples or subsamples are displayed as a regression line under **Samples** ▶ **Sample list** ▶ **Curves and data** ▶ **Linear regression**. The regression analysis contain all the subsamples of a sample that were created with the same versions of the operating procedure and of the methods.

Reprocessing regression analyses

Prerequisite:

- The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.

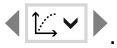
1 Selecting the sample or subsample

- Select a sample or subsample for which the regression line is to be displayed.
  If a sample is selected, the results for all subsamples of this sample with a statistical correlation will be displayed.
  If a subsample is selected, then only those results will be displayed which were available at the time of the determination of the subsample.

All the subsamples of a sample that were determined with the same versions of the operating procedure and of the methods are contiguous for the statistical evaluation.

2 Displaying the regression line

- Display the results of the regression analysis as a line under **Curves and data** ▶ **Linear regression** while a determination is running or after it has finished.

If there are multiple regression commands, the regression line for the corresponding command can be selected in the selection list  . The arrows to the right and left of the selection list are used to switch between the commands.
The version of the operating procedure used and the method in abbreviated form are output in the selection list in order to be able to distinguish between the determinations.

A table with information for each subsample that was included in the regression analysis is displayed under the regression lines. Subsamples with invalid values are not displayed in the regression lines, but are listed in the table.

3 Exclusion of data points

- Right-click to select the desired data point in the chart under **Curves and data** ▶ **Linear regression**.
  or
- Right-click to select the desired subsample in the table under **Curves and data** ▶ **Linear regression**.
- Select **Exclude** in the context menu.

The subsample is marked as an outlier and is no longer included in any regression analysis of the determination. The regression analysis is repeated.

4 Inclusion of excluded data points

- Right-click to select the desired data point in the chart under **Curves and data** ▶ **Linear regression**.
  or
- Right-click to select the desired subsample in the table under **Curves and data** ▶ **Linear regression**.
- Select **Include** in the context menu.

The excluded, marked subsample is included again in the regression analysis. The regression analysis is repeated.

See also

Displaying linear regression (chapter 5.10.12, page 344)

EVAL LINEAR REGRESSION – Parameters (chapter 5.11.8.68, page 776)

Reevaluating curves (chapter 5.10.11.7, page 335)

Reprocessing Sample statistics (chapter 5.10.13.2, page 352)

Reprocessing calculations (chapter 5.10.13.1.1, page 350)

5.10.13 Displaying the results

Prerequisite:

- The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.
  or
- The **Samples** ▶ **Search queries** subsection is opened. A search query is opened and at the front.

1 Selecting the subsample

- Select the subsample for which the results are to be displayed.

2 Displaying the results

- In **Results** ▶ **Raw data**, display the raw data that was recorded during a determination.
  or
- In **Results** ▶ **Predictions**, display the calculations for spectra that were made during a determination.
  or

- In **Results** ▶ **Calculations**, display the calculations that were made during a determination.
  or
- In **Results** ▶ **Sample statistics**, display the sample statistics that were created during a determination.
  or
- In **Results** ▶ **Monitoring**, display the monitoring that was created during a determination.

If there are multiple commands, the results for the corresponding command can be selected in the selection list . The arrows to the right and left of the selection list are used to switch between the commands.

See also

Copying table (chapter 5.2.8, page 172)

Reprocessing Sample statistics (chapter 5.10.13.2, page 352)

Reprocessing calculations (chapter 5.10.13.1.1, page 350)

5.10.13.1 Calculations – Definition

In **Samples** ▶ **Sample list** ▶ **Results** ▶ **Calculations**, the calculated results are displayed in a table which was created by the **CALC** commands for the selected subsample.

If a calculated result was created in the **CALC** command more than once (e.g. because the command is used in a **LOOP** command or because multiple commands with identical command names were used), only the last result that was calculated before cancellation is displayed in the **Calculations** subsection.

All the subsamples of a sample that were determined with the same versions of the operating procedure and of the methods are combined for the statistical evaluation.

If a calculation is carried out with the aid of a variable parallel to the command that generates the variable, then it is not mandatory for the **CALC** command to calculate the result with the end value of the variable, depending on the time sequence of the **CALC** command.

Overview list

The following data for the selected calculated result is shown in the overview list:

Name	Name of the result which was defined in the **CALC** command in **Properties** ▶ **Parameters**.
Result value	Numerical value of the calculated result.

Unit	Unit of the calculated result. The selected unit is used only for the informative presentation of the result in the formula editor and in reports. The unit has no influence on further calculations of the result.

If the **Calculate statistics** option was activated in the properties of the **CALC** command, then the following statistics values are also displayed in the corresponding columns:

Mean value	Mean value of the results of all the subsamples with a statistical correlation at the time of the determination.
s(abs)	Absolute standard deviation of the mean value of all statistically correlated subsamples at the time of determination.
s(rel)	Relative standard deviation of the mean value of all statistically correlated subsamples at the time of determination (absolute standard deviation in relation to the mean value).
n	Number of subsamples which were taken into account in the sample statistics at the time of the determination.

Further information regarding the variables used, the formula and the result saved as a variable is loaded and displayed by selecting the calculated result in the table in **Detail view**.

Variables whose value has changed more than once during the sequence are affected by the following behavior:

- For subsamples which have already been created in version 2.8 or earlier versions of the OMNIS Software, the following applies: The last value that this variable contained after the respective end of a determination of a subsample is displayed in **Detail view** ▶ **Variables used** and is available for further calculations.
- For subsamples which were created in version 2.9.0 or higher of the OMNIS Software, the following applies: The value of the variable actually used is displayed in **Detail view** ▶ **Variables used**.

See also

Filtering Search queries and Server search queries (chapter 5.10.2.3, page 246)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Reprocessing Sample statistics (chapter 5.10.13.2, page 352)

Reprocessing calculations (chapter 5.10.13.1.1, page 350)

5.10.13.1.1 Reprocessing calculations

In **Samples** ▶ **Sample list** ▶ **Results** ▶ **Calculations**, the results are displayed that were created by the **CALC** command for the selected subsample.

If a result was created in the **CALC** command more than once (e.g. because the command is used in a LOOP or because multiple commands with identical command names were used), only the last result is displayed in the **Calculations** subsection.

The results of canceled subsamples are also displayed in the table.

If a calculation is carried out with the aid of a variable parallel to the command that generates the variable, the **CALC** command calculates the result depending on the time sequence of the process and not necessarily with the end value of the variable.

Prerequisites:

- The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.

1 Selecting a subsample

- Select the subsample for which the calculations are to be reprocessed.

2 Displaying the results

- Display the calculation results of the subsample in **Results** ▶ **Calculations**.

  It depends on the command type which values are shown as results.

  If the **Calculate statistics** option was activated in the properties of the **CALC** command, the corresponding statistics values are displayed in the table.

3 Editing the calculation parameters

- Click on a result in the table.
- Click on $f(x)=$ to open the **Calculation parameters** window.
- Edit the calculation parameters as desired.

More information on the parameters: *(see "CALC – Parameters", chapter 5.11.8.64, page 768)*
The parameters **Result unit**, **Decimal places** and **Formula** can be recalculated.

The subsample with the reprocessed calculations is marked with .

All the subsamples with a statistical correlation that were determined with the same versions of the operating procedure and of the methods are also recalculated with the new parameters and marked with .
Subsamples which are statistically connected with signed subsamples cannot be reprocessed.

4 Discarding changes

- If you want to discard the changes, click on ↩ under **Results** ▶ **Calculations** ▶ **Calculation parameters**.

The calculation parameters will be reset to their original state.

5 Saving the sample list

- Save the sample list by clicking on 💾.

All the subsamples of the sample with a correlation are recalculated and their statistics is updated.

The subsample with the reprocessed calculations is marked with .

Further information regarding the variables used, the formula and the result saved as a variable is loaded and displayed by selecting the calculated result in the table in **Detail view**.

Variables whose value has changed more than once during the sequence are affected by the following behavior:

- For subsamples which have already been created in version 2.8 or earlier versions of the OMNIS Software, the following applies: The last value that this variable contained after the respective end of a determination of a subsample is displayed in **Detail view** ▶ **Variables used** and is available for further calculations.
- For subsamples which were created in version 2.9.0 or higher of the OMNIS Software, the following applies: The value of the variable actually used is displayed in **Detail view** ▶ **Variables used**.

See also

CALC – Parameters (chapter 5.11.8.64, page 768)

Displaying the results (chapter 5.10.13, page 347)

Reprocessing Sample statistics (chapter 5.10.13.2, page 352)

Reprocessing subsample data (chapter 5.10.7.5, page 283)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.13.2 Reprocessing Sample statistics

Statistics data for selected samples or subsamples are displayed under **Samples** ▶ **Sample list** ▶ **Results** ▶ **Sample statistics**. The sample statistics contain all the subsamples that were created with the same versions of the operating procedure and of the methods. If a sample consists of several subsamples with different operating procedures, separate sample statistics are calculated for each operating procedure.

Recalculating statistics

Prerequisites:

- The **Samples** ▶ **Sample lists** subsection is opened. A sample list is opened and at the front.

1 Selecting the sample or subsample

- Select the sample or subsample for which the sample statistics is to be reprocessed.

2 Displaying statistics data

- In **Results** ▶ **Sample statistics**, display the statistics data that were calculated during the determination for the selected sample or subsample.

If a subsample was selected, the data of all the subsamples with a statistical correlation are displayed in a table. This includes all the subsamples of the sample that were determined with the same versions of the operating procedure and of the methods.

Underneath the table, the mean value, the absolute and relative standard deviation as well as the population n of the subsamples with a correlation are displayed.

3 Excluding outliers from the sample statistics

- Right-click on the desired subsample in the table under **Results** ▶ **Sample statistics**.

- Select **Exclude** in the context menu.

The selected subsample is marked as an outlier and is no longer included in the sample statistics. When calculating mean values (e.g. for the titer), the subsample is ignored. The sample statistics are recalculated.

If results from subsamples are invalid, it is not possible to calculate the sample statistics and the corresponding entries in the table are displayed as **Invalid**. Once the subsample with the invalid results is deleted, the sample statistics are recalculated automatically.

4 Including outliers in the sample statistics

- Right-click on the desired subsample in the table under **Results** ▶ **Sample statistics**.
- Select **Include** in the context menu.

The subsample marked as outlier is included again in the sample statistics. The sample statistics are recalculated.

See also

Reprocessing calculations (chapter 5.10.13.1.1, page 350)

Reprocessing subsample data (chapter 5.10.7.5, page 283)

5.10.13.3 Reevaluating raw data

The raw data for the selected subsample is displayed under **Samples** ▶ **Sample list** ▶ **Results** ▶ **Raw data**. After the determination of a subsample has been executed, the results of certain commands can be reevaluated. This means that erroneous evaluations can be corrected.

Reevaluation of raw data is only available for subsamples that were determined with the **STDADD ISE dos** or **STDADD ISE auto** command.

Prerequisite:

- The **Results** ▶ **Raw data** subsection is opened. A sample list is opened and at the front.
- The determination with a **STDADD ISE dos** command or a **STDADD ISE auto** command was ended.

1 Selecting the subsample

- Select the subsample for which the raw data is to be shown.

The collected raw data for the subsample is displayed under **Results** ▶ **Raw data**.

2 Selecting the command

- Select the requested command in the selection list with . The arrows to the right and left of the selection list can be used to switch between the commands.

3 Opening the window Reevaluation

- Click on to open the **Reevaluation** window.

If a subsample or a command was selected for which no reevaluation is available, no parameters are displayed in the window. This also applies if no command was selected in the selection list and the overview over all the commands is displayed in the subsection.

4 Changing the evaluation parameters

- Change the evaluation parameters as needed.

As soon as the field in which the changes have been made is exited, the raw data is reevaluated with the modified parameters.

The subsample with the reevaluated raw data is marked with .

5 Discarding changes

- If you want to discard the changes, click on .

The evaluation parameters will be reset to the last saved state.

6 Saving changes

- Save changes by clicking on .

The subsample with the reevaluated raw data is marked with .

See also

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Recording subsamples (chapter 5.10.7.1, page 273)

Reprocessing calculations (chapter 5.10.13.1.1, page 350)

Subsamples – Statuses (chapter 5.10.7.3, page 276)

5.10.13.4 Monitoring – Definition

The selected variables, including the defined limit value pairs, which were defined in **Processes** ▶ **Operating procedures** ▶ **Properties** ▶ **Result monitoring** are listed in **Samples** ▶ **Sample list** ▶ **Results** ▶ **Monitoring**.

Overview list

The following data of the selected subsample is shown in the overview list:

Variable name	Name of the variable.
Value	Value of the variable.
Unit	Unit of the variable.
Status	Monitoring status.
Min. (warn.)	Defined lower warning limit.
Max. (warn.)	Defined upper warning limit.
Min. (control)	Defined lower control limit.
Max. (control)	Defined upper control limit.

See also

Filtering Search queries and Server search queries (chapter 5.10.2.3, page 246)

Filtering the monitoring status (chapter 5.10.13.4.2, page 357)

Result monitoring – Definition (chapter 5.11.1.11, page 408)

5.10.13.4.1 Result monitoring – Status

Monitored results that are shown in the **Sample list** are displayed with status icons. In addition, monitored results are also displayed in **Samples** **Sample list** **Results** **Monitoring** with their status icons.

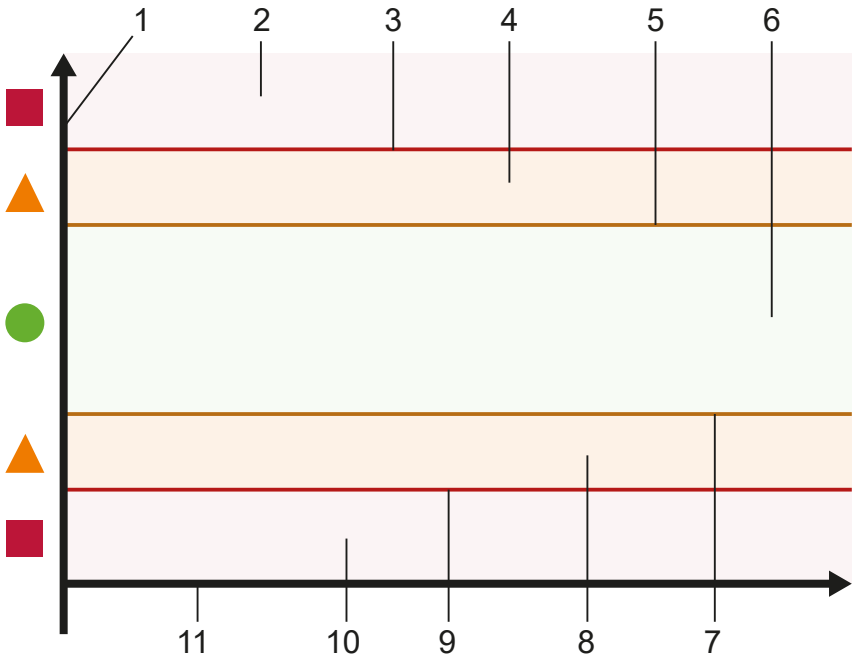
Depending on the defined limits, monitored results are displayed with the following status icons:

●	The value of the results or variables lies within the defined upper and lower **warning limits**.
▲	The value of the results or variables lies outside of the defined upper and lower **warning limits**, but within the defined upper and lower **control limits**.

The value of the results or variables lies outside of the defined upper and lower **control limits**.

The status icons of the values are adjusted when the results are recalculated.

Explanations regarding the monitored value ranges



1	**Result values (y-axis)** Distribution of the result quantities.
2	**Value range outside of the upper control limit** The values of this area all lie above the upper control limit. Mathematical representation:]upper control limit; ∞[
3	**Upper control limit** Defined upper control limit for the measured values.
4	**Value range outside of the upper warning limit** The values of this area all lie above the upper warning limit up until the upper control limit. Mathematical representation:]upper warning limit; upper control limit]
5	**Upper warning limit** Defined upper warning limit for the measured values.
6	**Area of validity (value range within warning limits)** The values of this area all lie within or up until the upper and lower warning limit. Mathematical representation: [upper warning limit; lower warning limit]

7	**Lower warning limit** Defined lower warning limit for the measured values.
8	**Value range outside of the lower warning limit** The values of this area all lie below the lower warning limit up until the lower control limit. Mathematical representation: **]**lower warning limit; lower control limit**]**
9	**Lower control limit** Defined lower control limit for the measured values.
10	**Value range outside of the lower control limit** The values of this area all lie below the lower control limit. Mathematical representation: **]**lower control limit; -∞**[**
11	**Time (x-axis)** Temporal course of the subsample measurements.

See also

Enabling monitoring (chapter 5.7, page 193)

Sensor – Properties (chapter 5.12.6.2, page 1001)

5.10.13.4.2 Filtering the monitoring status

When filtering, the search results under **Samples** ▶ **Sample list** ▶ **Results** ▶ **Monitoring** are included.

Filtering according to monitoring status

Prerequisites:

- Surveillance is activated.

1 Opening a search query

- In **Samples** ▶ **Search queries** select the desired search query and open it with a double-click.

2 Open the filter

- Open the filter by clicking on .

The area for selecting configurable filter criteria is opened.

3 Selecting a logical connective

- Select the logical connective **All filter criteria must be met** from the selection list.

Only search results matching all the selected filter criteria will be displayed in the list.

4 Add filter criterion

- Add additional filter criteria by clicking on .
- Select a filter criterion from the selection list.

5 Selecting the filter criterion

- Select the **Monitoring status** filter criterion.

6 Within the limits

- Select the **Equals** filter operator.
- Select the **Within the limits** status.
- Apply the selected filter criteria by clicking on **[Filter]**.

The search results shown are subsamples that contain monitored results within the warning limits (indicated by).

7 Warning limits violated

- Select the **Equals** filter operator.
- Select the **Warning limits violated** status.
- Apply the selected filter criteria by clicking on **[Filter]**.

The search results shown are subsamples that contain monitored results outside of the warning limits and/or outside of the control limits (indicated by or).

8 Control limits violated

- Select the **Equals** filter operator.
- Select the **Control limits violated** status.
- Apply the selected filter criteria by clicking on **[Filter]**.

The search results shown are subsamples that contain monitored results outside of the control limits (indicated by).

9 Filter criteria combination

- Select the **Equals** filter operator.
- Select the **Warning limits violated** status.
- Add additional filter criteria by clicking on .
- Select the **Does not equal** filter operator.
- Select the **Control limits violated** status.
- Apply the selected filter criteria by clicking on **[Filter]**.

The search results shown are subsamples that contain monitored results within the control limits, but outside of the warning limits (indicated by ▲).

To reset the filter or to delete or save it, perform steps 7 - 10 *(see "Filtering Search queries and Server search queries", chapter 5.10.2.3, page 246)*.

See also

Creating Search queries and Server search queries (chapter 5.10.2.2, page 244)

Monitoring – Definition (chapter 5.10.13.4, page 355)

Recording the result monitoring (chapter 5.11.1.11.1, page 408)

Result monitoring – Status (chapter 5.10.13.4.1, page 355)

Sample list – Tab (chapter 5.2.2, page 159)

Search queries – Definition (chapter 5.10.2, page 243)

User rights – Directory (chapter 4.5.7.4, page 89)

5.10.13.5 Predictions – Subsection

The predictions are displayed in tables which were created by the **PREDICT** commands for selected subsamples in **Samples** ▶ **Sample list** ▶ **Results** ▶ **Predictions**.

The results are displayed in the **Overview** area and can be re-evaluated and corrected in the **Reprocessing** area.

Overview area

All predictions are displayed in a table under **Overview**.

Sample information	The following information is displayed under Sample information:
▪ **Sample name**	▪ Name of the sample.
▪ **Subsample name**	▪ Name of the subsample.
Identification result	The following information is displayed under Identification result:
▪ **Identified as**	▪ If identification is successful, the name of the identified product or product group. ▪ If identification has failed, then the status of the identification is: **Unidentified** or **Ambiguous**.
Quantification results	The following information is displayed under Quantification results:

▪ **Reference parameter/unit**	▪ The result of a reference parameter with unit is displayed in a column. **Note**: If no unit has been defined, then only the reference parameter is displayed.
Verification result	The following information is displayed under Verification result:
▪ **Status**	▪ If verification is successful, then **Successful** will be displayed. ▪ If verification fails, then **Failed** is displayed.
	If the identification or verification has failed or if a model outlier has been detected, then the result will be marked with this red status icon.

Reprocessing area

The predictions can be reevaluated and corrected under **Reprocessing**. In addition, information on the name, version and object ID of the model is displayed that was used for the execution of the determination and for the reevaluation.

Additional information on reprocessing predictions: *(see "Reprocessing predictions", chapter 5.10.13.5.1, page 363)*.

Quantification model

If a quantification model and the slope/y-intercept correction in the **PREDICT** command correspond (name, version and object ID), then the predictions from various subsamples are grouped and displayed in tables.

The following information about the selected subsamples is shown in the table of a quantification model:

Sample name	Name of the sample.
Subsample name	Name of the subsample.
Calculated value	Value of the prediction that was determined by using the quantification model on the selected spectrum without the use of a slope/y-intercept correction.
	If a model outlier is detected, then the result will be marked with a red status icon.
Corrected value	Value of the prediction that was determined by applying the quantification model to the selected spectrum with the use of a slope/y-intercept correction. If no slope/y-intercept correction was used, then this corrected value is identical to the calculated value.

After selecting a quantification model under **Reprocessing** in the **Repredict with** field or selecting a slope/y-intercept correction in the **Correct with** field, the following information is also displayed in the table:

Old value	Numerical value of the original prediction. If a slope/y-intercept correction was used, then the corrected value is displayed.
New value	Numerical value of the repredicted prediction. If a slope/y-intercept correction was used, then the corrected value is displayed.
■	If a model outlier is detected, then the result will be marked with a red status icon.
Repredicted with	Name and version of the quantification model which was used to repredict the prediction.
Corrected with	Name of the slope/y-intercept correction with which the prediction was corrected. If no slope/y-intercept correction was used, then **No correction** is displayed.

Additional information on the used quantification model or the slope/y-intercept correction is displayed under **Reprocessing** in the **Detail view**.

Even before saving, the post-processed results are also displayed updated in the **Predictions** ► **Overview** area. If the changes are not saved afterwards, then they will be lost.

Identification model

If an identification model in the **PREDICT** command matches (name, version and object ID), then predictions from different subsamples will be displayed grouped in tables.

The following information on the selected subsamples is displayed in the table of an identification model:

Sample information	The following information is displayed under Sample information:
▪ **Sample name**	▪ Name of the sample.
▪ **Subsample name**	▪ Name of the subsample.
▪ **Expected product**	▪ Name of the expected product. **Note:** This information is displayed only if the identification model was used for verification.
Identification result	The following information is displayed under Identification result:
▪ **Identified as**	▪ If identification is successful, the name of the identified product or product group. ▪ If identification has failed, then the status of the identification is: **Unidentified** or **Ambiguous**.

▪ **Probability**	▪ The probability with which the spectrum was assigned to the expected product or to the expected product group. If the identification has failed, then **N/A** will be displayed.
Verification result	The following information is displayed under Verification result:
▪ **Status**	▪ If verification is successful, then **Successful** will be displayed. ▪ If verification fails, then **Failed** is displayed.
	If the identification or verification has failed, then the result will be marked with a red status icon.

Additional information on the identification model used is displayed under **Reprocessing** in the **Detail view**.

Model hierarchy

If a model hierarchy in the **PREDICT** command matches (name, version and object ID), then predictions from different subsamples will be displayed grouped in tables.

The following information on the selected subsamples is displayed in the table of a model hierarchy:

Sample information	The following information is displayed under Sample information:
▪ **Sample name**	▪ Name of the sample.
▪ **Subsample name**	▪ Name of the subsample.
▪ **Expected product**	▪ Name of the expected product. **Note:** This information is displayed only if the model hierarchy was used for verification.
Identification result	The following information is displayed under Identification result:
▪ **Identified as**	▪ If identification is successful, the name of the identified product or product group. ▪ If identification has failed, then the status of the identification is: **Unidentified** or **Ambiguous**.
▪ **Probability**	▪ The probability with which the spectrum was assigned to the expected product or to the expected product group. If the identification has failed, then **N/A** will be displayed.
Verification result	The following information is displayed under Verification result:
▪ **Status**	▪ If verification is successful, then **Successful** will be displayed. ▪ If verification fails, then **Failed** is displayed.

	If the identification or verification has failed, then the result will be marked with a red status icon.
Quantification result (Name of reference parameter)	The quantification result is shown in the Reprocessing area with the name and the unit of the reference parameter. The following information is displayed under the reference parameter:
▪ **Calculated value**	▪ Value of the prediction that was determined by using the quantification model on the selected spectrum without the use of a slope/y-intercept correction.
▪ **Corrected value**	▪ Value of the prediction that was determined by applying the quantification model to the selected spectrum with the use of a slope/y-intercept correction. If no slope/y-intercept correction was applied, then this corrected value is identical to the calculated value.

Additional information on the model hierarchy used is displayed under **Reprocessing** in the **Detail view**.

See also

Displaying the results (chapter 5.10.13, page 347)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

Models – Definition (chapter 5.13.1.1, page 1056)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

Reprocessing predictions (chapter 5.10.13.5.1, page 363)

Slope/y-intercept correction – Definition (chapter 5.13.2.6, page 1124)

5.10.13.5.1 Reprocessing predictions

Under **Samples** ▶ **Sample list** ▶ ▶ **Results** ▶ **Predictions** in the **Overview** and **Reprocessing** areas, the results are displayed that were created by the **PREDICT**-command for the selected subsamples.

Instructions for the reprocessing of quantification results

Prerequisite:

- The **Samples** ▶ **Sample lists** subsection is opened.
- The **Results** ▶ **Predictions** ▶ **Reprocessing** subsection is opened in the open sample list.
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting subsamples

- Select the subsamples in the sample list that are to be reprocessed.

Additional information on multiple selection in the sample list: *(see "Editing sample list", chapter 5.10.1.2, page 212)*

The calculated values of the selected samples are displayed in the **Overview** and **Reprocessing** areas.

2 Reprocessing results

- The following options are available for reprocessing in the **Reprocessing** area:
  - In the **Repredict with** field, select the quantification model with which the results are to be repredicted.
  - In the **Correct with** field, select the slope/y-intercept correction with which the results are to be corrected.
  - Fill in both of the above fields, if both a reprediction with a new quantification model and a slope/y-intercept correction are to be carried out.

The following information is also displayed in the table: **Old value**, **New value**, **Repredicted with** and **Corrected with**. In addition, results that were determined as model outliers are marked with the red status icon .

More information on the information in the table: *(see "Predictions – Subsection", chapter 5.10.13.5, page 359)*

Additional information on the used quantification model or the slope/y-intercept correction are displayed in the table under **Detail view**.

Even before saving, the post-processed results are also immediately displayed updated in the **Predictions** ▶ **Overview** area. If the changes are not saved afterwards, they will be lost.

3 Saving sample list

- Save the sample list by clicking on .

The subsamples with repredicted predictions are marked with .

See also

CALC – Parameters (chapter 5.11.8.64, page 768)

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Creating identification model (chapter 5.13.3.4, page 1139)

Creating quantification model (chapter 5.13.1.7, page 1074)

Displaying the results (chapter 5.10.13, page 347)

Editing identification model (chapter 5.13.3.5, page 1141)

Editing quantification model (chapter 5.13.1.12, page 1082)

Editing sample list (chapter 5.10.1.2, page 212)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

Publishing models (chapter 5.13.1.11, page 1080)

5.10.14 System variables – Definition

A system variable is a variable that is defined in the **Samples** work area by the user and it can then be used within the whole system in various methods and operating procedures.

See also

Creating system variables (chapter 5.10.14.2, page 366)

Samples – Actions (chapter 5.10, page 208)

Sorting the overview list (chapter 5.2.7, page 171)

5.10.14.1 System variables – Subsection

The following functions are available in **Samples** ► **System variables**:

- $(x)_+$

  Create system variable is used to create a new system variable for use throughout all commands and methods.

-

  Use **Save** to save all changes.

-

  The view is reloaded with **Update view**. Unsaved entries are reset to the last saved version.

-

  Delete system variable deletes the system variable.

Overview list

The following information is displayed in the overview list:

Name	Name of the system variables. The name can be modified after clicking in the name field of the system variable.
Type	Type of the system variables (number or text).

Value	Numerical value or text content of the system variables.
Unit	Physical unit of the system variables.
Saved	Time at which the system variable was last saved.
Variable name	Names of the created system variables under which the variables can be used in the formula editor.

See also

Creating system variables (chapter 5.10.14.2, page 366)

5.10.14.2 Creating system variables

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The **System variables** subsection in the **Samples** work area is opened.

Creating system variables

1 Setting up system variable

- The following options are available for creating a system variable:
  - Create a new line by clicking on $(x)_+$.
  - Right-click on a line to open the context menu and select **[Create system variable]**.
  - Create a new line with the key combination **[CTRL]**+**[I]**.

2 Naming system variable

- In the name field for the new system variable, enter the desired name.

Each name can be assigned only once (upper/lower case is not taken into account).
The texts in the input field can be copied, inserted, or cut using the context menu.

The designation with which the variables are used in the formula editor is displayed in the **Variable name** field.

3 Entering values

- Select **Number** or **Text** from the selection list in the **Type** field.
- Enter a numerical value or text of the system variables in the **Value** field.
- As an option, enter the physical unit of the system variables in the **Unit** field.

4 Saving system variable

- The following options are available for saving a system variable:
  - Save the system variable by clicking on .
  - Save the system variable with the key combination **[CTRL]**+**[S]**.

The date and the time the system variables were saved are displayed in the **Saved** field.

Deleting system variable

1 Selecting system variable

- Select the system variable by clicking on the number at the beginning of the line.

2 Deleting system variable

- The following options are available for deleting a system variable:
  - Click on to delete the selected system variable.
  - Right-click on the highlighted line to open the context menu and select **[Delete]**.
  - Click the **[DELETE]** key to remove the selected system variable.

Once a system variable is renamed or deleted, this variable is no longer available in commands, methods and operating procedures. A determination that requires that system variable cannot be carried out correctly until that variable is recreated as system variable with the original name or until it is replaced by another variable.

See also

Samples – Definition (chapter 5.10.4, page 251)

Sorting the overview list (chapter 5.2.7, page 171)

System variables – Definition (chapter 5.10.14, page 365)

5.10.15 Control chart – Definition

Control charts describe with the help of a chart how subsample data behaves over a time period in the OMNIS Software. The chart shows the variance of all subsamples included in the sample list and highlights outliers predefined by the user. The **Control chart** is created by means of a statistical sample survey of **Subsample data** from one or more **Sample lists**.

Control charts are created and managed in **Samples** ▶ **Control charts**.

During creation, the center line as well as the respective lower and upper warning limits, control limits and specification limits can be defined. An action defined in the operating procedure that is automatically executed when a limit is exceeded can be selected.

Additional information on creating and editing a control chart:
(see "Creating and editing a control chart", chapter 5.10.15.2, page 369)
Additional information on the control chart diagram:
(see "Control chart – Area", chapter 5.10.15.3, page 373)

See also

Control chart – Area (chapter 5.10.15.3, page 373)

Control chart – Properties (chapter 5.10.15.4, page 375)

Control chart – Tab (chapter 5.10.15.5, page 376)

Control charts – Subsection (chapter 5.10.15.1, page 368)

Creating and editing a control chart (chapter 5.10.15.2, page 369)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Subsample data – Definition (chapter 5.11.1.10, page 403)

5.10.15.1 Control charts – Subsection

The following functions are available in **Samples** ▶ **Control charts**:

-

  Create control chart creates a new control chart in which statistical samples from selected sample lists are drawn. A user-defined variable from an existing operating procedure is used as the y-axis. In the overview list, an already existing control chart can be opened with a double-click.
-

  Use **Delete control charts** to delete the selected control charts from the database.

Overview list

The following information is displayed in the overview list:

Name	Name of the control chart. The name can be adjusted after opening the control chart.
Saved	Time at which the control chart was last saved.
Version	Version number of the control chart. A new version is created automatically each time the control chart is saved.

See also

Control chart – Definition (chapter 5.10.15, page 368)

Control chart – Tab (chapter 5.10.15.5, page 376)

Creating and editing a control chart (chapter 5.10.15.2, page 369)

5.10.15.2 Creating and editing a control chart

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Creating or editing a control chart

- Create a new control chart in **Samples** ▶ **Control charts** by clicking on .

A dialog for setting the control chart opens.

To edit an existing control chart. select the required control chart from the overview list in **Samples** ▶ **Control charts** and open it by double-clicking on the control chart name. Click on to open the settings of the selected control chart.

2 Setting a control chart

- Enter the required name for the control chart in the **Name of the control chart** field. A maximum of 255 characters is allowed.

- Fill in the following information in the **Control chart data** column:
  - Select the operating procedure that contains the variable to be controlled from the **Operating procedure** selection list.
  - Select the variable to be controlled in the **Variable** field. Only the variables contained in the selected operating procedure are displayed.
  - Select the sample list from which the data will be read from the **Sample list** selection list. All suitable sample lists are selected by default.
- Fill in the following information in the **Control chart setup** column:
  - Select the desired type of control chart from the **Type of the control chart** selection list.
  - Add a label to the axis in the **Label of the y-axis** field (max. 255 characters). This label is displayed in the control chart.

- Fill in the following information in the **Statistical sample survey** column:
  - Define the statistical sample frequency in the **Statistical sample frequency** field. An integer between **1** and **999** must be entered as a value or selected by clicking on the arrow. If 1 is input, then every statistical sample will be entered. If higher values are entered, the statistical sample survey is restricted (e.g. with 2 only every second sample is entered, with 3 only every third sample is entered, etc.). The default value resets the statistical sample frequency to 1.
  - Enable the **Start date** check box to define the start date. The **Start date** field can thus be edited and the desired start date can be selected. By default, the current date is inserted. If required, a past date can also be selected as the start date.
  - To define the end date, enable the **End date** check box. The **End date** field can thus be edited and the desired end date can be selected. If required, a past date can also be selected as the end date.
  - To display only the samples of the last [n] days, enable the **Setting the [n] days/subsamples** check box, where [n] stands for the number of days. The selection list and the input field can thus be edited. By default, only the data of the last day (n = 1) is displayed.
    To display only the last [n] samples, enable the **Setting the [n] days/subsamples** check box where [n] is the number of samples. The selection list and the input field can thus be edited. By default, only the data of the last sample (n = 1) is displayed.

If a **statistical sample frequency** filter and **Data of the last [n] days** or **Data of the last [n] subsamples** are used simultaneously, the last [n] filter is used first.

Either a date range or a specification of the last [n] subsamples or [n] days can be specified. Activating one of these specifications automatically deactivates the other.

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

Click on **[Next]** to open another dialog for setting the limit values in the control chart.

3 Defining limit values

- Select the mean value from the **Center line** selection list:
  - X bar/mean value
  - Enter value
- When enabling the **Warning limits** check box, fill out the following information in **Warning limits** column:
  - In the **Upper warning limit** field, set the upper warning limit or No Limit in the control chart.
  - In the **Lower warning limit** field, set the lower warning limit or No Limit in the control chart.
  - Select the action of the operating procedure from the **Action (if outside range)** selection list that is to be carried out if the result is outside of the warning limits.
- When enabling the **Control limits** check box, fill out the following information in **Control limits** column:
  - In the **Upper control limit** field, set the upper control limit or No Limit in the control chart.
  - In the **Lower control limit** field, set the lower control limit or No Limit in the control chart.
  - Select the action of the operating procedure from the **Action (if outside range)** selection list that is to be carried out if the result is outside of the control limits.
- When enabling the **Specification limits** check box, fill out the following information in **Specification limits** column:
  - In the **Upper specification limit** field, set the upper specification limit or No Limit in the control chart.
  - In the **Lower specification limit** field, set the lower specification limit or No Limit in the control chart.
  - Select the action of the operating procedure from the **Action (if outside range)** selection list that is to be carried out if the result is outside of the specification limits.

In order to be available in the selection list, the actions must be defined in the operating procedure as a sequence for the limit violation.

In the selection list for the upper and lower warning limits, a single, double or triple standard deviation can be selected instead of a standard value or user-defined value.

Click on **[Create]** or **[Save]** to enter the control chart on the tab and save it.

See also

Control chart – Definition (chapter 5.10.15, page 368)

Control chart – Properties (chapter 5.10.15.4, page 375)

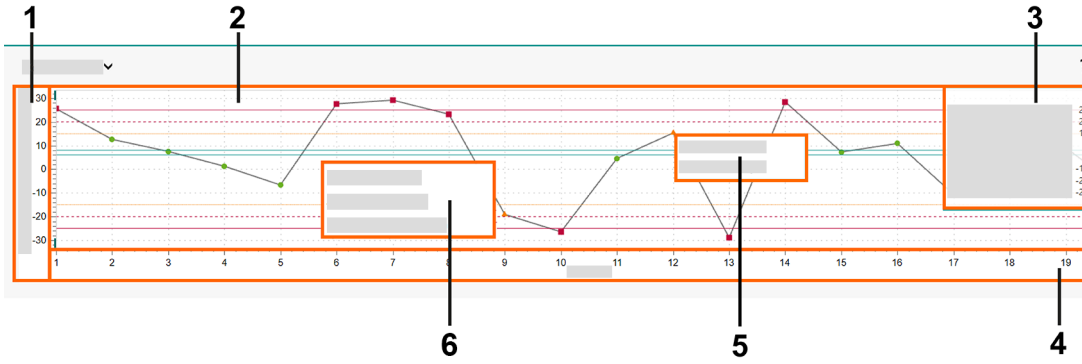
Control chart – Tab (chapter 5.10.15.5, page 376)

Control charts – Subsection (chapter 5.10.15.1, page 368)

5.10.15.3 Control chart – Area

The control chart is displayed as a diagram based on the selected sample data in **Sample** ▶ **Control charts** ▶ **Control chart**. The chart shows all subsample data and can be configured by the user to illustrate specific parts of the chart in more detail.

The data points of the chart can be updated even if the determination of the sample data has not yet been completed.



1 **y-axis command variable**
Shows the values of the selected command variable on the y-axis of the chart.

2 **Chart area**
Shows the complete control chart by means of a chart. The control chart is dynamic and supports different zoom levels. Use the mouse wheel or a selection rectangle to adjust the zoom level of the control chart. The view can be moved with the right mouse button. **Reset view** restores the default view. Click on one of the **data points** in the chart or under sample data to highlight the selected data point in both windows.

3 Legend
The **legend** shows the values of the defined limits and center line. The legend can be shown and hidden.

4 x-axis subsample number
Shows the subsample number on the x-axis of the chart.

5 Data point context menu
Right-click on a **data point** in the **chart area** to open a context menu. The selected data point can be included or excluded from the control chart in the **Data point context menu**.

6 Chart area context menu
Right-clicking in the **chart area** opens a context menu. The chart can be copied, the view can be reset and the legend can be shown and hidden in the **Chart area context menu**. The chart can be copied into an external document with the "Copy chart" option.

Table 2 Chart elements - center line and limit lines

	Shows the **center line** or the **user-defined center line**.
	Shows the **warning limit**, if defined.
	Shows the **control limit**, if defined.
	Shows the **specification limit**, if defined.

Table 3 Chart elements - Data points

	The data point is within all defined limits.
	The data point is outside the warning limits.
	The data point is outside the control limits.

See also

Control chart – Definition (chapter 5.10.15, page 368)

Control chart – Tab (chapter 5.10.15.5, page 376)

Creating and editing a control chart (chapter 5.10.15.2, page 369)

5.10.15.4 Control chart – Properties

Click on in **Samples** ▶ **Control charts** ▶ **Control chart** to open the **Properties** window. The following information is available in the **General** subsection:

Name	Name of the control chart.
Object ID	Identification number of the control chart.
Version	Version number of the control chart. A new version is created automatically each time a control chart is saved.
Created	Time at which the control chart was created.
Created by	User ID of the user who created the control chart.
Saved	Time at which the control chart was last modified.
Saved by	User ID of the user who last modified the control chart.

See also

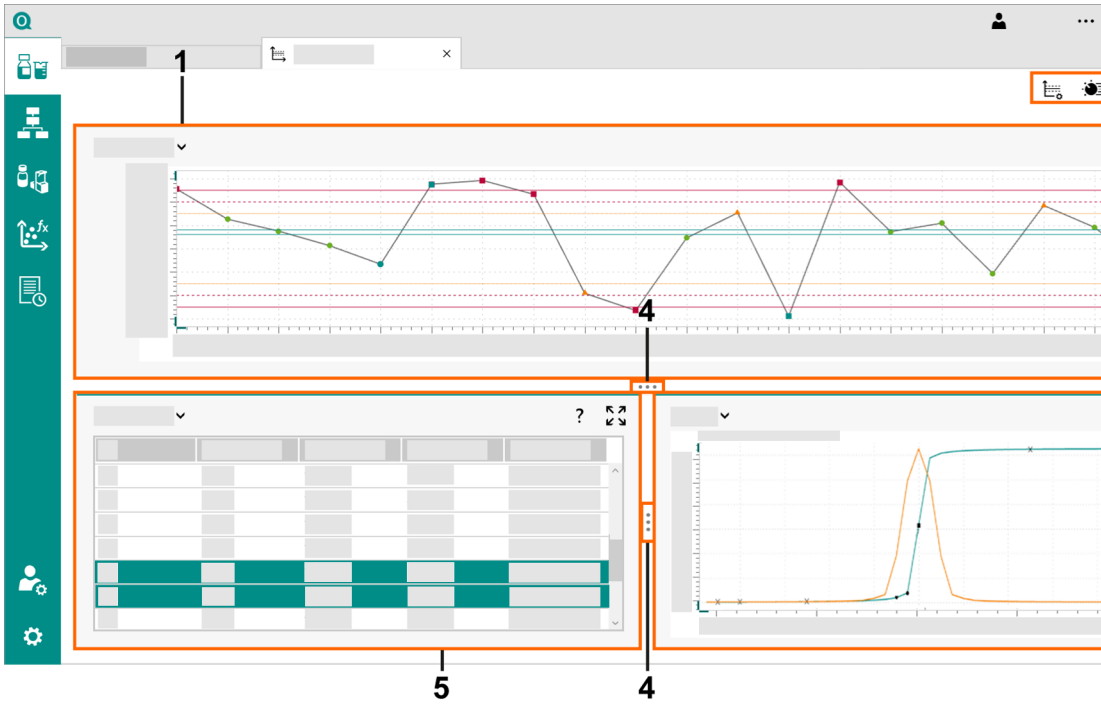
Control chart – Area (chapter 5.10.15.3, page 373)

Control chart – Tab (chapter 5.10.15.5, page 376)

Control charts – Subsection (chapter 5.10.15.1, page 368)

Creating and editing a control chart (chapter 5.10.15.2, page 369)

5.10.15.5 Control chart – Tab



1 Control chart
Shows the control chart created from the sample data. Additional information on the functions of the control chart: *(see "Control chart – Area", chapter 5.10.15.3, page 373)*

2 Toolbar
Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

3 Curves
Shows the individual curves of the sample data. The curves can only be displayed but not changed.

4 Divider
The size of the individual areas can be adjusted with the divider.

5 Sample data
Shows the required **Sample data** to create the control chart. Additional information on the sample data area: *(see "Sample data – Area", chapter 5.10.15.6, page 377)*

See also

Control chart – Definition (chapter 5.10.15, page 368)

Control charts – Subsection (chapter 5.10.15.1, page 368)

Creating and editing a control chart (chapter 5.10.15.2, page 369)

Sample data – Area (chapter 5.10.15.6, page 377)

5.10.15.6 Sample data – Area

The sample data of the control chart is displayed under **Samples** ▶ **Control charts** ▶ **Sample data**.

If the values of the samples displayed in the control chart have changed in the meantime, then the view of the control chart can be updated by clicking on .

The following information is displayed under Sample data:

Table 4

No.	Number of the sample with which it was included in the control chart.
Sample name	Name of the sample with which it was included in the control chart from the sample list.
Subsample name	Name of the subsample with which it was included in the control chart from the sample list.
Command variable	The value of the selected command variable.
Determination start	Time point at which the subsample determination was started.

See also

Control chart – Definition (chapter 5.10.15, page 368)

Control chart – Tab (chapter 5.10.15.5, page 376)

Control charts – Subsection (chapter 5.10.15.1, page 368)

Creating and editing a control chart (chapter 5.10.15.2, page 369)

5.11 Processes – Actions

In the **OMNIS Stand-Alone**, the following actions can be executed in the subsections of the **Processes** work area:

- Operating procedures are created, processed, signed and managed in **Processes** ▶ **Operating procedures**.
- Methods are created, processed, signed and managed in **Processes** ▶ **Methods**.

In the **OMNIS Client/Server system**, the following actions can be executed in the subsections of the **Processes** work area:

- Operating procedures are created, processed, signed, managed, published and withdrawn in **Processes** ▶ **Operating procedures**.
- Methods are created, processed, signed, managed, published and withdrawn in **Processes** ▶ **Methods**.
- Published operating procedures are downloaded from the OMNIS Server in **Processes** ▶ **Server operating procedures**.
- Published methods are downloaded from the OMNIS Server in **Processes** ▶ **Server methods**.

Further information on the actions in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Creating a signature (chapter 5.8.1, page 198)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Creating and editing tags (chapter 5.9.1, page 203)

Deleting a signature (chapter 5.8.3, page 201)

Method – Definition (chapter 5.11.3, page 413)

Methods – Subsection (chapter 5.11.3.1, page 414)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Server method – Definition (chapter 5.11.4, page 425)

Server methods – Subsection (chapter 5.11.4.1, page 426)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Server operating procedures – Subsection (chapter 5.11.2.1, page 412)

Tags – Definition (chapter 5.9, page 203)

User rights – Directory (chapter 4.5.7.4, page 89)

5.11.1 Operating procedure – Definition

Information on operating procedures in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

An **operating procedure** defines the work sequence for the analysis of subsamples. This work sequence is defined using **methods** and device-independent **commands** that can be aligned sequentially and in parallel.

Prerequisite for the use of an operating procedure:

- The associated methods have at least one **work system** assigned.

Subsample data can be assigned to an operating procedure (e.g., information such as sample size, analysis date, rack position, etc.).

The operating procedures are created and managed in **Processes ▶ Operating procedures**. The operating procedures are assigned to the subsamples in **Samples ▶ Sample profiles**. The operating procedures can also be assigned directly to a subsample on the tab of a sample list in **Samples ▶ Sample lists**.

The operating procedures are saved under a freely selectable name. A new **version** is created each time a change is saved. A Comment can be added to each operating procedure.

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Command – Properties (chapter 5.11.8.1, page 431)

Creating a signature (chapter 5.8.1, page 198)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Creating and editing tags (chapter 5.9.1, page 203)

Deleting a signature (chapter 5.8.3, page 201)

Method – Definition (chapter 5.11.3, page 413)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Report template – Directory (chapter 5.10.1.4.1, page 233)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Subsample data – Definition (chapter 5.11.1.10, page 403)

User rights – Directory (chapter 4.5.7.4, page 89)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.1.1 Operating procedures – Subsection

Information on the operating procedures in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The following functions are available in **Processes** ► **Operating procedures**:

-

  Use **Create operating procedure** to create a new operating procedure in which methods and commands can be inserted and edited.

-

  Use **Import operating procedures** to import one or multiple OPRO files (**O**MNIS **Pro**cess) as operating procedures. If the operating procedures contain methods, models, model hierarchies or slope/y-intercept corrections, then these will also be imported. In order to import the work systems contained in the methods, the check box must be enabled for the import.

-

  Use **Export operating procedures** to export each selected operating procedure as an OPRO file (**O**MNIS **Pro**cess). If the operating procedures contain methods, models, model hierarchies or slope/y-intercept corrections, then these will also be exported. In order to export the work systems contained in the methods, the check box **Export with work system** must be enabled for the export.
-

  Use **Create report** to create a report for the selected operating procedure. The reports can be saved as a PDF file or also printed out.
-

  Duplicate operating procedures duplicates the selected operating procedures under the same name and with a consecutive number. If a name already ends with a number, then this number is incremented by +1. The newly created operating procedures contain the same methods, commands and parameters as the original operating procedures.
-

  The properties of the selected element are displayed in the **Properties** window.
-

  Use **Delete operating procedures** to delete all selected operating procedures from the database. Methods contained in the operating procedures are retained in the database.
  Note: Only applicable in **OMNIS Stand-Alone**.
-

  Use **Remove operating procedures from local OMNIS Client** to remove the selected operating procedures from the local system. If non-published operating procedures have been selected, then they will be permanently deleted. If selected operating procedures have been published, then they will be retained on the OMNIS Server. Methods contained in the operating procedures are retained in both cases.
  Note: Applicable only in the **OMNIS Client/Server system**.

Operating procedures can be filtered by names and tags. Additional information on filtering operating procedures: *(see "Filtering tags", chapter 5.9.2, page 206)*

Overview list

The following information is displayed in the overview list:

Name	Name of operating procedure. The name can be modified after opening the operating procedure.

Published	Status of the operating procedure in the **OMNIS Client/Server system**. Additional information: *(see "Operating procedures and methods – Status", chapter 5.11.1.8, page 401)* **Note**: Applicable only in the **OMNIS Client/Server system**.
Saved	Time at which the operating procedure was last saved.
Version	Version number of the operating procedure. A new version is created automatically each time the operating procedure is saved.
Tags	Existing tags assigned to this operating procedure.
Data permissions	Existing data permissions assigned to this operating procedure. **Note**: Applies only if data permissions are enabled and the user has the necessary user rights.

See also

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Data permissions – Definition (chapter 4.5.9, page 105)

Exporting operating procedures and methods (chapter 5.11.1.5, page 393)

Importing operating procedures and methods (chapter 5.11.1.4, page 392)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Operating procedure and method – Tab (chapter 5.2.5, page 168)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedure – Properties (chapter 5.11.1.2, page 383)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Restoring operating procedure and associated methods (chapter 5.11.1.9, page 402)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.1.2 Operating procedure – Properties

Information on operating procedures in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Clicking on under **Processes** ▶ **Operating procedures** opens the **Properties** window within an operating procedure. Depending on the selected element, the following functions and information are available in the 7 subsections **General**, **Parameters**, **Execute with**, **Result monitoring**, **Reports**, **Export** and **Web exports**:

General

Depending on the selection (**Operating procedure**, **Method** or **Command**), other information is listed:

Name	Name of operating procedure, method or command. Can be edited for the operating procedure and commands within the operating procedure (max. 255 characters).
Object ID	Identification number of the operating procedure, method or command.
Version	Version number of the operating procedure or method. A new version is created automatically each time an operating procedure or method is saved.
Created	Time at which the operating procedure or method was created.
Created by	Person who created the operating procedure or method.
Saved	Time at which the operating procedure or method was last changed.
Saved by	Person who changed the operating procedure or method.
Index	Index of the method, how often it is contained in the operating procedure.
Comment	Comment on the operating procedure, method or command. (editable, max. 255 characters).

Parameters

If the entire **Operating procedure** is selected, then the **Subsample data** can be defined and edited.

If a **Method** is selected, then the **Method variables** defined in the method can be displayed and their values can be edited.

If a **Command** within the operating procedure is selected, then the command parameters can be edited. If a command within a **Method** is selected, then the command parameters can only be displayed and cannot be edited.

Execute with

If the **Operating procedure** is selected, then the following functions are available:

Prevent determination with expired equipment	If this check box is enabled, then determinations with expired equipment will be prevented. This makes it possible to ensure that determinations are made only with equipment that is still within its defined **Working life** or **Validity period**. The **Working life** or **Validity period** must be defined and monitoring must be enabled for this to be effective. The determination can then be started only if the user has been assigned the **Start determinations with expired equipment** user right. Additional information on the activation of monitoring:*(see "Enabling monitoring", chapter 5.7, page 193)*
Reserve work systems only when needed	If this check box is enabled, then work systems can be selected that will not be reserved until later during the determination. With this, a determination can already be started, even if some functional units of these work systems are still reserved by other determinations. After the activation, the work systems that are assigned to a method within the operating procedure are displayed. Work systems that are assigned exclusively to a method in an optional run, are not displayed. Additional information on the user-defined reservation behavior: *(see "Configuring a parallel determination", chapter 5.10.8.5, page 301)*

If the **Method** is selected, then the work systems assigned to the method are displayed. The following functions are available:

Release work system after completing the method	If this check box is enabled, the assigned work system is released as soon as the selected method has ended. This allows for the work system to be used in an operating procedure that runs in parallel. After activation, the following specific parameter is displayed: ▪ **Skip optional runs (error/stop) with a new reservation of work systems** Additional information on the user-defined reservation behavior: *(see "Configuring a parallel determination", chapter 5.10.8.5, page 301)*
Skip optional runs (error/stop) with a new reservation of work systems	If this check box is enabled, the optional runs **Execute on error** and **Execute on stop** are skipped if these reserved a work system that had already been released. This avoids that the defined behavior in case of an error or stop is executed for a work system that has already been released and is being used in another run. If enabled, then this setting applies not only for all run sequences of this type within the separate methods, but also within the entire operating procedure.

If the **Command** within a method is selected, then the functional units assigned to the command are displayed.

Result monitoring

Clicking on **[Monitor results]** allows result monitoring to be defined and edited. Additional information on the result monitoring:*(see "Recording the result monitoring", chapter 5.11.1.11.1, page 408)*

Reports

Reports can be generated automatically after the completion of a determination. A new report can be defined by clicking on . can be used to delete a report definition once again. Additional information on the generation of reports: *(see "Creating report", chapter 5.10.1.4, page 224)*

This function is used for automated report generation following the completion of a determination. The **REPORT** command is suitable for creating reports during a determination. More information on the **REPORT** command: *(see "REPORT – Parameters", chapter 5.11.8.76, page 793)*

Exports

Exports can be created automatically after a determination has been finished. A new export can be defined by clicking on . can be used to delete an export definition once again. Additional information on exporting: *(see "Exporting subsample data", chapter 5.10.1.3, page 220)*

This function is used for automated export generation following the completion of a determination. The **EXPORT** command is suitable for the creation of exports during a determination. More information on the **EXPORT** command: *(see "EXPORT – Parameters", chapter 5.11.8.69, page 780)*

Web exports

Web exports, during which the subsample data is sent to a web API, can be created automatically after a determination has been finished. A new web export can be defined by clicking on . can be used to delete a web export definition once again. Additional information on the web export: *(see "Sending data to third-party software", chapter 5.10.7.8, page 291)*

This function is used for automated web export generation following the completion of a determination. The **CALL WEB API** command is suitable for the creation of web exports during a determination. Additional information on the **CALL WEB API** command: *(see "CALL WEB API - Parameter", chapter 5.11.8.65, page 771)*

See also

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

EXPORT – Parameters (chapter 5.11.8.69, page 780)

Editing subsample data (chapter 5.11.1.10.1, page 404)

Formula editor – Brief description (chapter 5.11.9, page 825)

Method – Properties (chapter 5.11.3.2, page 416)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Parallel determination – Run (chapter 5.10.8.4, page 299)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

REPORT – Parameters (chapter 5.11.8.76, page 793)

Result monitoring – Definition (chapter 5.11.1.11, page 408)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.1.3 Creating and editing an operating procedure

Information on operating procedures in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Creating a new operating procedure

- In **Processes** ▶ **Operating procedures**, click on .

A tab opens with the newly created operating procedure and the title **New operating procedure**.

To edit an existing operating procedure, select the desired operating procedure from the list in **Processes** ▶ **Operating procedures** and open it by double-clicking on the operating procedure name.

2 Naming or renaming an operating procedure

- Click on

.
- Click on to open the **Properties** window.
or
- Double-click on

to open the **Properties** window directly.
- Enter the desired name in the **Name** field under **Properties** ▶ **General**.

The following characters are not allowed: **. | ' " { }**

3 Entering a comment (optional)

- Enter the desired comment in the **Comment** field under **Properties** ▶ **General**.

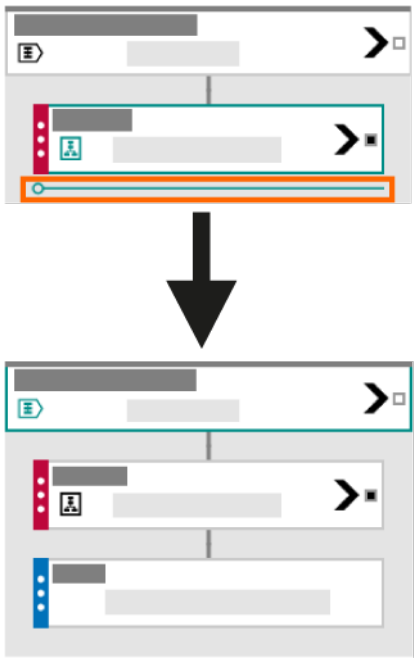
An operating procedure containing a Comment is indicated with in the operating procedures editor.

4 Inserting methods and commands

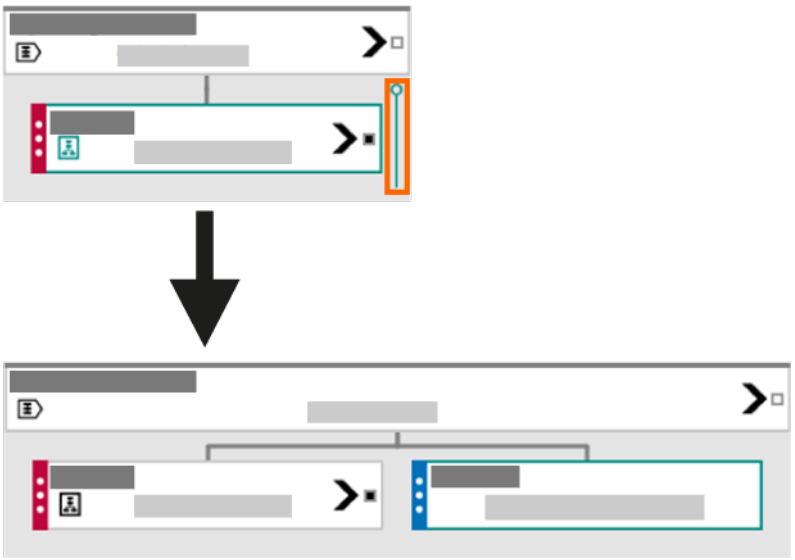
- Click on to open the **Library** window.
- Use drag and drop to insert the desired methods into the operating procedure in **Library** ▶ **Methods**.
- Use drag and drop to insert the desired commands into the operating procedure in **Library** ▶ **Commands**.

The methods and commands can be inserted either one below the other or side by side:

- Commands and methods that are aligned one below the other are executed **sequentially**. A green horizontal line shows the insertion position of an object.



- Commands and methods that are aligned side by side are executed in **parallel**. A green vertical line shows the insertion position of an object.



- A command or a method can be inserted repeatedly in the same operating procedure. Commands and methods are automatically indexed to ensure that the nomenclature remains unambiguous.

The following options are available for inserting and editing commands and methods:

- Commands and methods can be moved within the operating procedure using drag and drop or can be removed from the operating procedure by clicking on ✕.
- Commands can be copied from operating procedures or methods with **[CTRL]**+**[C]** and inserted in other operating procedures or methods with **[CTRL]**+**[V]**.
- Device-dependent commands can be inserted only into methods, but not into operating procedures.
- Methods cannot be edited in the operating procedures editor. In order to edit it, the method must be opened in the method editor.

5 Inserting optional runs

- Click on to open the **Library** window.

- Use drag and drop to insert the desired optional run into the operating procedure in **Library** ▶ **Optional runs**.
- Insert the desired methods or commands in the optional run.

An optional run can be inserted only parallel to the run. Additional information on the optional runs:

(see "Run in case of a stop – Definition", chapter 5.11.6, page 428)

(see "Run in case of an error – Definition", chapter 5.11.5, page 427)

(see "Run in case of a limit value violation – Definition", chapter 5.11.7, page 429)

6 Editing command parameters

- Select the desired command.
- Click on to open the **Properties** window.
- Change the desired command parameter in **Properties** ▶ **Parameters**.

7 Editing subsample data

- Click on .
- Click on to open the **Properties** window.
- Select the **Properties** ▶ **Parameters** subsection.
- Define the subsample data that is inserted automatically into the sample list when the operating procedure is used.

8 Defining result monitoring

- Click on .
- Click on to open the **Properties** window.
- Select the **Properties** ▶ **Result monitoring** subsection.
- Define result monitoring according to the instructions in *(see "Recording the result monitoring", chapter 5.11.1.11.1, page 408)*.

9 Defining reports

- Click on .
- Click on to open the **Properties** window.
- Select the **Properties** ▶ **Reports** subsection.

- Define the reports according to the instructions in *(see "Creating report", chapter 5.10.1.4, page 224)*.

10 Defining exports

- Click on

.
- Click on to open the **Properties** window.
- Select the **Properties** ► **Exports** subsection.
- Define the exports according to the instructions in *(see "Exporting subsample data", chapter 5.10.1.3, page 220)*.

11 Saving the operating procedure

- Click on to save the operating procedure. The operating procedure is automatically validated during saving.

The operating procedure is saved. The version and change date of the operating procedure are updated automatically in the **Properties** ► **General** subsection.

In the **OMNIS Client/Server system**, an operating procedure can be published after saving it. Information on publishing operating procedures: *(see "Publishing the operating procedure and the method", chapter 5.11.1.6, page 396)*

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

Editing subsample data (chapter 5.11.1.10.1, page 404)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.1.4 Importing operating procedures and methods

Information on importing operating procedures and methods in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- At least one OMNIS process file (***.opro**) is available.

1 Selecting operating procedures or methods

- Click on to open the **Import data** window in **Processes ► Operating procedures** or **Processes ► Methods**.

2 Browsing for folder

- Select the folder where the desired operating procedures or methods are saved.

3 Selecting the file

- Select the OMNIS process files or enter the names of the OMNIS process files in the **File name** field.

4 Importing work systems (optional)

- If the operating procedures or methods contain work systems, then these can also be imported if required. To accomplish this, enable the **Import with work system** check box.

Import with work system imports all existing **Solution conditions** and **Sensor conditions**. Depending on the command, these are stored in the method and defined for the functional unit of the work system. Exactly the same Work system must be used as in the imported operating procedure or method in order to have the conditions also be taken into account at the time of the execution of the imported operating procedure or method. If the original Work system is replaced by another Work system, then the defined **Solution conditions** and **Sensor conditions** are lost.

If the **Work system** used in the imported operating procedure or method already exists in the OMNIS Software, then it is automatically assigned to the imported operating procedure or method, even if the **Import with work system** check box is disabled and the existing **Solution conditions** and **Sensor conditions** are taken into account.

5 Confirming and importing the selection

- Click **[Open]** to confirm the selection.

The operating procedures or methods are imported into the OMNIS Software.

If the operating procedures or methods contain models, slope/y-intercept corrections or model hierarchies, then these will also be imported.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Defining solution conditions and sensor conditions (chapter 5.12.7.4, page 1020)

Exporting operating procedures and methods (chapter 5.11.1.5, page 393)

Importing the templates (chapter 3.2, page 11)

Method – Definition (chapter 5.11.3, page 413)

Methods – Subsection (chapter 5.11.3.1, page 414)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

5.11.1.5 Exporting operating procedures and methods

Information on exporting operating procedures and methods in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- At least one operating procedure or method is available in the overview list.

1 Selecting operating procedures or methods

- Select the required operating procedures or methods in **Processes** ▶ **Operating procedures** or **Processes** ▶ **Methods** and click on to open the **Export data** window.

2 Selecting an export option

- Enable the **Selected operating procedures** or **Selected methods** check box to export all of the operating procedures or methods highlighted in the overview list.
- Enable the **All operating procedures** or **All methods** check box to export all operating procedures or methods from the overview list.

3 Exporting work systems (optional)

- If the operating procedures or methods contain work systems, then these can also be exported if required. To do this, enable the **Export with work system** check box.

Solution conditions and **Sensor conditions** are always exported. Depending on the command, these are stored in the method and defined for the functional unit of the work system.

4 Selecting or entering a target folder

- Select the target folder or enter the absolute path in the address bar where the selected operating procedures or methods are to be saved as OPRO files.

5 Confirming and exporting the selection

- Click on **[Export]** to confirm the selection. Depending on the selection, one or more OPRO files are exported under the respective names of the operating procedures or methods. Click on **[Open target folder]** to open the target folder.

The files are saved under the name of the respective operating procedure or method. If the name of the operating procedure or method contains one of the special characters > < : " / \ | * ? or CON, PRN, AUX, NUL, COM1 … COM9, LPT1 … LPT9, then these will be replaced by the character **(_)**.

If the operating procedures or methods contain models, slope/y-intercept corrections or model hierarchies, then these will also be exported.

All time indications are converted into Coordinated Universal Time (UTC±00:00) when exporting. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.
The local time on the computer is used for the date and time displayed in the file name.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Defining solution conditions and sensor conditions (chapter 5.12.7.4, page 1020)

Importing operating procedures and methods (chapter 5.11.1.4, page 392)

Method – Definition (chapter 5.11.3, page 413)

Methods – Subsection (chapter 5.11.3.1, page 414)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.1.6 Publishing the operating procedure and the method

Operating procedures and methods can be published in the **OMNIS Client/Server system**.

Publishing an operating procedure

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The **OMNIS Client/Server system** is set up.
- The connection to the OMNIS Server is available.

1 Selecting an operating procedure

- Create a new operating procedure. *(see "Creating and editing an operating procedure", chapter 5.11.1.3, page 387)*
  or
- In **Processes** ▶ **Operating procedures**, select an existing operating procedure and open it with a double-click.

A tab with the newly created or the selected operating procedure opens.

2 Calling up the dialog

- Open the **Publish operating procedure** dialog by clicking on .
- In the **Name suffix** field, enter the required name suffix for the operating procedure that is to be published.

The following special characters must not be used: . | ' " { }
The name suffix is added only to the selected operating procedure.
The field for the name of the operating procedure is pre-filled and cannot be edited.

3 Publishing an operating procedure

- Click on **[Publish]** to publish the operating procedure.

The published operating procedure is marked by in **Processes** ▶ **Operating procedures** and **Server operating procedures**. When an operating procedure is published, the associated methods and work systems are also published.

When publishing an operating procedure that contains the **ADD TO SAMPLE LIST** command, the referenced operating procedures and associated methods are also published and the sample data is applied from the referenced sample profile.

If the operating procedure contains data permission and this is to be displayed to another user group with different data permissions, then the published operating procedure must be published once more. This creates a new server operating procedure.

Available data permissions for an operating procedure that has already been published can be changed in the overview list under **Processes** ► **Operating procedures**. The data permissions are updated for the corresponding server operating procedure and this does not create a new server operating procedure. Additional information on data permissions: *(see "Assigning data permissions", chapter 4.5.9.2, page 112)*

Published operating procedures are automatically synchronized with the OMNIS Server. They are available in the overview list under **Processes** ► **Server operating procedures** for all connected OMNIS Clients and are protected against changes. They must first be downloaded in order to be subsequently used for a determination. Further information on the server operating procedures: *(see "Server operating procedure – Definition", chapter 5.11.2, page 410)*

A published operating procedure is a copy of the unpublished operating procedure. The unpublished operating procedure is retained under **Processes** ► **Operating procedures** without changes.

When publishing, the name change of the operating procedure, addition or removal of a method, command or work system is taken into account. The changed operating procedure is published.

An operating procedure cannot be signed until it has been published and all associated methods have been signed. If an operating procedure that has already been signed is to be published, the signature must first be deleted and then added again after publication. Further information on the signature in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

A published operating procedure can be withdrawn on the **Processes** ► **Operating procedures** tab to restrict its use. Further information on withdrawing operating procedures: *(see "Withdrawing operating procedure and method", chapter 5.11.1.7, page 400)*

Publishing a method

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The **OMNIS Client/Server system** is set up.
- The connection to the OMNIS Server is available.

1 Selecting a method

- Create a new method. *(see "Creating and editing a method", chapter 5.11.3.3, page 418)*
  or
- In **Processes** ▶ **Methods**, select an existing method and open it with a double-click.

A tab with the newly created or the selected method opens.

2 Publishing a method

- Publish the method by clicking on .

The published method is marked by in **Processes** ▶ **Methods** and **Server methods**. When a method is published, the associated work systems, models, model hierarchies, and slope/y-intercept corrections are also published.

When publishing a method that contains the **ADD TO SAMPLE LIST** command, the referenced operating procedures and associated methods are also published and the sample data is applied from the referenced sample profile.

If the method contains data permission and this is to be displayed to another user group with different data permissions, then the published method must be published once more. This creates a new server method.

Available data permissions for a server method that has already been published can be changed in the overview list under **Processes** ▶ **Methods**. The data permissions are updated on the respective server method and this does not create a new server method. Additional information on data permissions: *(see "Assigning data permissions", chapter 4.5.9.2, page 112)*

Published methods are automatically synchronized with the OMNIS Server. They are available in the overview list under **Processes** ▶ **Server methods** for all connected OMNIS Clients and are protected against changes. They must first be downloaded in order to use them. Further information on the server methods: *(see "Server method – Definition", chapter 5.11.4, page 425)*

A published method is a copy of the unpublished method. The unpublished method is retained under **Processes** ▶ **Methods** without changes.

When publishing, the name change of the method, addition or removal of a command or work system is taken into account. The modified and newly saved method is published.

Only a published method or method can be signed. If a method that has already been signed is to be published, the signature must first be deleted and then added again after publication. Further information on the signature in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

A published method can be withdrawn on the **Processes** ▶ **Methods** tab to restrict its use. Further information on withdrawing methods: *(see "Withdrawing operating procedure and method", chapter 5.11.1.7, page 400)*

See also

Creating a signature (chapter 5.8.1, page 198)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Method – Definition (chapter 5.11.3, page 413)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Server method – Definition (chapter 5.11.4, page 425)

Server methods – Subsection (chapter 5.11.4.1, page 426)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Server operating procedures – Subsection (chapter 5.11.2.1, page 412)

User rights – Directory (chapter 4.5.7.4, page 89)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.1.7 Withdrawing operating procedure and method

If the use of a published operating procedure or method by connected OMNIS Clients should be limited, the published operating procedure or method can be withdrawn.

Prerequisite:

- The **OMNIS Client/Server system** is set up.
- The connection to the OMNIS Server is available.
- The user has the necessary rights. Further information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting the published operating procedure or method

- In **Processes** ▶ **Operating procedures** or **Methods**, select the desired published operating procedure or method and open it with a double-click.

A tab with the selected operating procedure or method opens.

A published operating procedure or method is marked in the overview list with .

2 Withdrawing a published operating procedure or method

- Withdraw the published operating procedure or method by clicking on .

The selected operating procedure or method is withdrawn. The withdrawn operating procedure or method is marked in the overview list with . A withdrawn operating procedure or method can only be used for the determination of subsamples if the **Start determinations with unreleased operating procedures** right is activated.

If an operating procedure is withdrawn, the associated methods remain published and can be used by the connected OMNIS Clients.
If a method is withdrawn, the operating procedures that contain it are marked with in the overview lists.
If the connection to the OMNIS Server is interrupted, the operating procedure or method is only withdrawn once the connection is established again.

A withdrawn operating procedure or method can be deleted from the OMNIS Server. Further information on deleting server operating procedures and server methods: *(see "Server operating procedures – Subsection", chapter 5.11.2.1, page 412)*, *(see "Server methods – Subsection", chapter 5.11.4.1, page 426)*

See also

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Server method – Definition (chapter 5.11.4, page 425)

Server methods – Subsection (chapter 5.11.4.1, page 426)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Server operating procedures – Subsection (chapter 5.11.2.1, page 412)

User rights – Directory (chapter 4.5.7.4, page 89)

5.11.1.8 Operating procedures and methods – Status

In the **OMNIS Client/Server system**, each operating procedure and method that is on the OMNIS Server has a status. This is displayed under **Processes** ▶ **Operating procedures** or **Server operating procedures** and **Methods** or **Server methods** in the **Published** column.

Published	Meaning
	Published The operating procedure or method is published.
	Contains withdrawn or deleted methods The operating procedure contains at least one withdrawn or deleted method.
	Withdrawn The operating procedure or method has been withdrawn.

The necessary rights must be enabled before an operating procedure or method can be used in a determination. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

If the operating procedures or methods are not published in **Processes** ▶ **Operating procedures** or **Methods**, then the **Published** column will be empty.

See also

Determination – Definition (chapter 5.10.8, page 295)

Determination – Preparation and follow-up (chapter 5.10.8.10, page 313)

Method – Definition (chapter 5.11.3, page 413)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Preparing determination (chapter 5.10.8.9, page 310)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Server method – Definition (chapter 5.11.4, page 425)

Server operating procedure – Definition (chapter 5.11.2, page 410)

User rights – Directory (chapter 4.5.7.4, page 89)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.1.9 Restoring operating procedure and associated methods

Information on the operating procedure and method in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Opening a sample list

- In **Samples** ▶ **Sample lists**, select the required sample list and open it with a double-click.

2 Selecting a subsample

- Select the subsample whose operating procedure and associated methods are to be restored.

3 Restoring operating procedure and methods

- In **Subsample** ▶ **Process**, click on .

The operating procedure and its associated methods are restored and can be used in the **Processes** work area.

If the restored operating procedure contains models, model hierarchies and slope/y-intercept corrections, then these will also be restored.

The required work systems and their functional units must be assigned to the associated methods in order to use the operating procedure once again for a determination. Furthermore, used variables must be referenced correctly.
The references between the name of the operating procedure and the variables used or between the method name and the variables used must be corrected if required (e.g. **SKIP** and method variables). The simplest course of action is to reset the names of the operating procedure and methods back to the original names.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Importing operating procedures and methods (chapter 5.11.1.4, page 392)

Method – Definition (chapter 5.11.3, page 413)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

Models – Definition (chapter 5.13.1.1, page 1056)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Sample list – Tab (chapter 5.2.2, page 159)

5.11.1.10 Subsample data – Definition

The **subsample data** defined in the operating procedure in **Processes** ▶ **Operating procedure** ▶ **Properties** ▶ **Parameters** (name, start of determination, weight, volume, etc.) simplifies the recording of subsamples with identical data. If a new subsample is created with an operating procedure in which subsample data is defined, then this subsample data will automatically be inserted into the sample list along with

its default values. In the sample list only the data that is to be changed now needs to be edited.

The subsample data is also available as '**Name**.*CurrentSubsampleData*' variables in the formula editor.

See also

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Editing subsample data (chapter 5.11.1.10.1, page 404)

Importing subsample data (chapter 5.10.7.7, page 289)

5.11.1.10.1 Editing subsample data

Information on the sample profile in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Opening an operating procedure

- Click in **Processes** ▶ **Operating procedures** to open a new operating procedure.
  or
- In **Processes** ▶ **Operating procedures**, select the required operating procedure and open it with a double-click.

A new tab with the new or the selected operating procedure opens.

2 Opening the subsample data

- Click on to open the **Properties** window.
  or
- Double-click on the operating procedure icon to open the **Properties** window directly.

The subsample data defined for the operating procedure is displayed in **Properties** ▶ **Parameters**.

2 entries are already available by default:

- **Name** field
  Field for displaying the name of the subsample in the sample list. The **Subsample** default value can be changed; the field, however, cannot be deleted.
- **Determination start** field
  Field for displaying the point in time at which the determination of the subsample was started.

3 Adding subsample data

- Click on to add additional subsample data or, alternatively, right-click in the text field and select **[Add input field]**.

A new input field is added to the right of the subsample data.

To delete subsample data, right-click in the text field and select **[Delete input field]**.

4 Defining subsample data

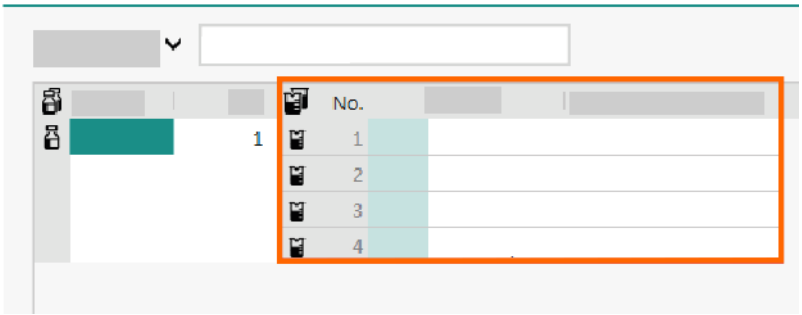
- In the **Field name short** field, enter the name for the input field that should be used as column header in the sample list.
- In the **Field name long** field, enter the name for the input field that is to be used as a designation in reports.
  Note: If no name is entered in the **Field name long** field, then the name in the **Field name short** field will be used in the reports.
- Select the required type (**Text**, **Number**, **Date** or **Selection list**) for the information in the **Type of input field** field.

- Select the required mode of use for the input field in the **Use as** field:
  - **Input field**: Field in which the user can enter data (for the **Text** or **Number** type).
  - **Result**: Field that can be filled with the corresponding commands during the determination run (**CALC** and **REQUEST**) (for when type = **Text** or **Number**). This field cannot be edited directly by the user.
  - **Sample size**: Input field for the sample size (for type = **Number**).
  - **Rack**: Input field or selection list for use as the variable in the **Rack/Park** field of the **MOVE TO RACK** command (for type = **Text** or **Selection list**).
  - **Sample position**: Input field for use as the variable in the **Position on the rack** field of the **MOVE TO RACK** command (for type = **Number**).
  - **Determination start**: Automatically completed field for the date and time of the determination start (for type = **Date**).
  - **User-defined selection list**: Selection list with which users can select a list element from a list they have defined themselves (for type = **Selection list**).
- Depending on the type and use of the input field, additional fields are displayed in the **Properties input field** section that can be filled out as required:
  - For fields of the **Text** type: **Default value**
  - For fields of the **Number** type: **Default value**, **Minimum value**, **Maximum value**, **Unit**
  - For fields of the **Selection list** type: **List elements**, **Default value**
- Enable the **Allow free text** check box to give users the option of creating a list entry themselves in the sample list if the predefined entries are not sufficient. This option is visible only if **Selection list** and **Rack**, **User-defined selection list** or **Solution** have been selected.
- Disable the **Editable field** check box if the user should not be able to edit the input field for the subsample in the sample list.
- Enable the **Allow empty field** check box if a field without the entry of a value is to be permissible.
- Enable the **Force entry** check box if the entry of a value is to be forced for empty fields before the determination is started. This option is visible only if **Allow empty field** has been enabled.

The **Properties input field** section is not available in the following cases:

- If **Text** or **Number** was selected in **Type of input field** and if **Result** was selected in **Use as**.
- If **Date** was selected in **Type of input field** and if **Determination start** was selected in **Use as**.

The names of the sample data that were defined in the operating procedure in the **Field name short** field are displayed as column headers in the sample list as soon as subsamples are recorded with this operating procedure.



5 Modifying the sequence of subsample data (optional)

- Select the required input field by clicking an editable field and move it to the left by clicking or move it to the right by clicking .

6 Saving subsample data

- Click on to save the operating procedure.

See also

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Recording samples (chapter 5.10.4.1, page 251)

Recording weighing data (chapter 5.10.7.4, page 280)

5.11.1.11 Result monitoring – Definition

Result monitoring is used to monitor selected variables during an analysis.

2 differing pairs of limit values can be defined for each monitored variable. In addition, an action can be selected respectively that will be carried out automatically once the value of the variable is exceeded or is fallen below.

Result monitoring is defined by clicking on **[Monitor results]** in **Processes** ▶ **Operating procedure** ▶ **Properties** ▶ **Result monitoring**.

The results are shown during analysis in **Samples** ▶ **Sample list** ▶ **Results** ▶ **Monitoring**.

See also

NOTIFY – Parameters (chapter 5.11.8.72, page 787)

Recording the result monitoring (chapter 5.11.1.11.1, page 408)

Run in case of a limit value violation – Definition (chapter 5.11.7, page 429)

5.11.1.11.1 Recording the result monitoring

1 Opening an operating procedure

- In **Processes** ▶ **Operating procedures**, click on to create a new operating procedure.
  or
- In **Processes** ▶ **Operating procedures**, select the desired operating procedure and open it with a double-click.

A new tab with the new or the selected operating procedure opens.

2 Opening the Result monitoring window

- Click on **[Monitor results]** in **Processes** ▶ **Operating procedure** ▶ **Properties** ▶ **Result monitoring**.

The **Result monitoring** window opens.

3 Add result monitoring

- Click on to add a new result monitoring.

4 Selecting a variable

- Click on to open the selection window for the variable that is to be monitored.
- Find the required variable with the 2 fields **Variable category** and **Subcategory**.

- Select the desired variable in the **Search result** field.
- Click on **[Apply]** to apply the selected variable.

The variables found in the search result can be limited further by entering a filter term. To accomplish this, enter the desired text that is to be contained in the variable name in the field above the list of found variables. The display is continuously updated.

The selection window for the variable is closed. The name of the selected variable is displayed in the **Variable** field.

5 Defining decimal places

- In the **Number of decimal places** field, enter the desired number of decimal places that is to be applied to all values in the defined result monitoring.

By default, 2 decimal places are used.

6 Defining warning limits

- Define the limits of the result monitoring in the **Lower warning limit**, **Upper warning limit**, **Lower control limit** and **Upper control limit** fields.
- The entries can be numeric values or formulas. Only formulas that return a numeric value are valid. Under **Subsample data** or **Sample data** the Type of input field **Text** can be selected and under Use as **Result** can be chosen, if the result returns a numeric value.
  - The **Time** function must not be used.

Rules for entering limit values:

- At least one limit value pair must be defined.
- The upper value of a limit value pair must be greater than the lower value.
- Furthermore, the value range of a limit value pair must lie within or outside of the second limit value pair on both sides.

If the validation does not correspond to the **rules for entering limit values**, this result monitoring cannot be carried out. However, the determination is not stopped.

7 Selecting an action

- Select the action from the selection list that is to be carried out if the result is outside of the limits.

If a limit value is exceeded or fallen below, a defined action can be triggered.

At least one **Optional Run** **Execute on limit** must be defined in order for an action to be able to be selected.

8 Saving result monitoring

- Click on to save the operating procedure.

If formulas are used for limit values, they will not be evaluated until during the execution of the determination.

If the selected variable contains an invalid value while the determination is being carried out, this will be processed the same as if the limit value was exceeded.

If a control limit is defined, it will be processed the same as if a limit value pair was exceeded, otherwise it will be processed the same as if the warning limit was exceeded.

See also

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Filtering Search queries and Server search queries (chapter 5.10.2.3, page 246)

Monitoring – Definition (chapter 5.10.13.4, page 355)

NOTIFY – Parameters (chapter 5.11.8.72, page 787)

5.11.2 Server operating procedure – Definition

A **Server operating procedure** is understood to be an operating procedure that is located on the OMNIS Server and is thus available to all connected OMNIS Clients.

A server operating procedure defines the work sequence for the analysis of subsamples. This work sequence is defined using **Server methods** and device-independent **commands** that can be aligned sequentially and in parallel.

Prerequisite for the use of a server operating procedure:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The server operating procedure has already been downloaded and is available under **Processes** ▶ **Operating procedures**. The associated server methods, work systems, models, model hierarchies slope/y-intercept corrections, solution conditions, and sensor conditions are also downloaded and listed in the corresponding subsections when a server operating procedure is downloaded.

A server operating procedure can be downloaded under **Processes** ▶ **Server operating procedures** by clicking on .
When downloading a subsample from a server search query, the associated server operating procedure is automatically downloaded.

- The associated methods have at least one **work system** assigned.

After downloading, all functional units of the published work system must be replaced by functional units from custom devices via drag-and-drop and the work system must be saved. No additional functional units can be added to a published work system, nor can any functional units be removed from it.

The published server operating procedures that were downloaded can be assigned to the subsamples on the tab of a sample list in **Samples** ▶ **Sample profiles** or **Samples** ▶ **Sample lists**.

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Server method – Definition (chapter 5.11.4, page 425)

Server operating procedures – Subsection (chapter 5.11.2.1, page 412)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.2.1 Server operating procedures – Subsection

The following functions are available under **Processes** ▶ **Server operating procedures**:

-

  Download operating procedures downloads the selected operating procedures with the associated methods, work systems, models, model hierarchies, and slope/y-intercept corrections. The downloaded operating procedures and the associated methods, work systems, models, model hierarchies and slope/y-intercept corrections are listed in the corresponding subsections and can be used.
-

  Update view updates the list of the server operating procedures. All entries are reloaded.
-

  The selected server operating procedures are deleted with **Delete server operating procedures**. To be able to delete the server operating procedures, these must first be withdrawn. If server operating procedures are deleted, then the server methods associated with it are not deleted. The deleted operating procedures are retained locally in the status **withdrawn** on the OMNIS Clients which downloaded the server operating procedures before they were deleted.

Server operating procedures can be filtered by names and tags. Additional information on filtering server operating procedures: *(see "Filtering tags", chapter 5.9.2, page 206)*

Overview list

The following information is displayed in the overview list:

Name	Name of the server operating procedure.
Published	Status of the server operating procedure in the **OMNIS Client/Server system**. Additional information: *(see "Operating procedures and methods – Status", chapter 5.11.1.8, page 401)* **Note**: Applicable only in the **OMNIS Client/Server system**.
Saved	Time at which the server operating procedure was last saved.
Version	Version number of the server operating procedure. A server operating procedure always has the version number 1.

Tags	Existing tags assigned to this server operating procedure.
Data permissions	Existing data permissions assigned to this server operating procedure. **Note**: Applies only if data permissions are enabled and the user has the necessary user rights.

See also

Data permissions – Definition (chapter 4.5.9, page 105)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Server methods – Subsection (chapter 5.11.4.1, page 426)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.3 Method – Definition

Information on the method in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

A **method** is understood to be a combination of commands that can be aligned sequentially and in parallel.

Prerequisite for the use of a method:

- At least one **work system** must be assigned to the method.
- The method must be contained in an **operating procedure**.

The methods are created and managed in the **Processes** work area. The methods are assigned to the operating procedures subsamples in **Processes ▶ Operating procedure**. The methods are saved under a freely selectable name. A new **version** is created each time a change is saved. There is no limit to the number of times saved methods can be used in various operating procedures at the same time. A Comment can be added to each method.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Methods – Subsection (chapter 5.11.3.1, page 414)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Server method – Definition (chapter 5.11.4, page 425)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.3.1 Methods – Subsection

Information on the methods in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The following functions are available in **Processes** ► **Methods**:

-

  Use **Create method** to create a new method in which commands can be inserted and edited.
-

  Use **Import methods** to import one or multiple OPRO files (**O**MNIS **Pro**cess) as methods. If the methods contain models, model hierarchies or slope/y-intercept corrections, then these will also be imported. In order to import the work systems contained in the methods, the check box must be enabled for the import.
-

  Use **Export methods** to export the methods as an OPRO file (**O**MNIS **Pro**cess). Use **Selected methods** to export all selected methods in the overview list. Use **All methods** to export all methods in the overview list. If the methods contain models, model hierarchies or slope/y-intercept corrections, then these will also be exported. In order to export the work systems contained in the methods, the check box **Export with work system** must be enabled for the export.
-

  Use **Create report** to create a report for each selected method. The reports can be saved as a PDF file or also printed out.

-

  Duplicate method duplicates the selected methods under the same name and with a consecutive number. If a name of a method already ends with a number, then this number is incremented by +1. The newly created methods contain the same commands, parameters, and optional runs as the original methods.

-

  The properties of the selected element are displayed in the **Properties** window.

-

  Use **Delete methods** to delete all selected methods from the database. If one of the methods is used in an operating procedure, then this method will be displayed in the operating procedure crossed out in red. In order to execute the operating procedure, all of the methods crossed out in red must be deleted from operating procedure.
  Note: Only applicable in **OMNIS Stand-Alone**.

-

  Use **Remove methods from local OMNIS Client** to remove the selected methods from the local system. If the non-published methods have been selected, then they will be permanently deleted. If selected methods have been published, then they will be retained on the OMNIS Server. If one of the methods is used in an operating procedure, then this method will be displayed in the operating procedure crossed out in red. In order to execute the operating procedure, all of the methods crossed out in red must be deleted from operating procedure. Server operating procedures that contain the removed method remain unchanged.
  Note: Applicable only in the **OMNIS Client/Server system**.

Methods can be filtered by names and tags. Additional information on filtering methods: *(see "Filtering tags", chapter 5.9.2, page 206)*

Overview list

The following information is displayed in the overview list:

Name	Name of the method. The name can be modified after opening the method.
Published	Status of the method in the **OMNIS Client/Server system**. Additional information: *(see "Operating procedures and methods – Status", chapter 5.11.1.8, page 401)* **Note**: Applicable only in the **OMNIS Client/Server system**.

Saved	Time at which the method was last saved.
Version	Version number of the method. A new version is created automatically each time the method is saved.
Tags	Existing tags assigned to this method.
Data permissions	Existing data permissions assigned to this method. **Note**: Applies only if data permissions are enabled and the user has the necessary user rights.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

Data permissions – Definition (chapter 4.5.9, page 105)

Exporting operating procedures and methods (chapter 5.11.1.5, page 393)

Importing operating procedures and methods (chapter 5.11.1.4, page 392)

Method – Definition (chapter 5.11.3, page 413)

Method – Properties (chapter 5.11.3.2, page 416)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Operating procedure and method – Tab (chapter 5.2.5, page 168)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Restoring operating procedure and associated methods (chapter 5.11.1.9, page 402)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.3.2 Method – Properties

Information on the method in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Clicking on under **Processes** ▶ **Method** within an opened method opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 3 subsections **General**, **Parameters** and **Execute with**:

In the Properties window in the method overview in **Processes** ▶ **Method**, instead of the 3 subsections that are described in the following, only the subsection **Signatures** is available.

General

Name	Name of the method (editable, max. 255 characters).
Object ID	Identification number of the method.
Version	Version number of the method. A new version is created automatically each time a method is saved.
Created	Time at which the method was created.
Created by	User ID of the user that created the method.
Saved	Time at which the method was last modified.
Saved by	User ID of the user that modified the method.
Comment	Comment on the method (editable, max. 255 characters).

Parameters

Method-specific variables can be defined as **method variables** in this subsection. These method variables are used for entering the formula under the **method variables** variable category and they can be found in the operating procedures which contain this method.

Further information on creating method variables: *(see "Creating a method variable", chapter 5.11.3.4, page 424)*

Execute with

In this subsection, you can define with which work systems the method is permitted to be executed. Only one work system can be used per method at the runtime of a determination. This work system is selected automatically by the OMNIS Software.

If the required functional units are available in the work system and these functional units can be uniquely assigned, the functional units in the work system are assigned to individual commands automatically. If several functional units of the same type are available, then the system is not able to uniquely assign the functional unit. In such cases, the desired functional unit has to be assigned to the command manually.

Further information on assigning functional units: *(see "Assigning a functional unit to a command", chapter 5.12.3.3, page 905)*

Signatures

The **Signatures** subsection is only available in the properties under **Processes** ▶ **Method**.

All the signatures available for the selected method are displayed in this subsection.

Additional information on signatures:

- *(see "Creating a signature", chapter 5.8.1, page 198)*
- *(see "Deleting a signature", chapter 5.8.3, page 201)*
- *(see "Displaying signatures", chapter 5.8.2, page 200)*
- *(see "Signature – Brief description", chapter 5.8, page 197)*

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Creating and editing a method (chapter 5.11.3.3, page 418)

Method – Definition (chapter 5.11.3, page 413)

Methods – Subsection (chapter 5.11.3.1, page 414)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Variables – Directory (chapter 5.11.9.3, page 827)

5.11.3.3 Creating and editing a method

1 Creating a new method

- In **Processes** ▶ **Methods**, click on .

A tab opens with the newly created method and the title **New method**.

To edit an existing method, select the required method from the list in **Processes** ▶ **Methods** and open it by double-clicking on the method name.

2 Naming or renaming the method

- Click on

.
- Click on to open the **Properties** window.
or
- Double-click on

to open the **Properties** window directly.
- Enter the desired name in the **Name** field under **Properties** ▶ **General**.

The following characters are not allowed: **. | ' " { }**

3 Entering a comment (optional)

- Enter the desired comment in the **Comment** field under **Properties** ▶ **General**.

A method containing a Comment is indicated by in the method editor, operating procedures editor, and library.

4 Assigning work systems

- Activate the check box for the method to assign the desired work systems in **Properties** ▶ **Execute with**.

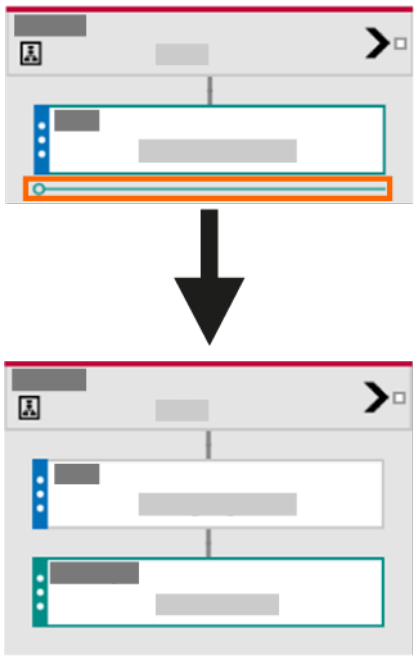
You should select only work systems which can be used to execute the method. This step can also be executed after inserting the commands.

5 Inserting commands

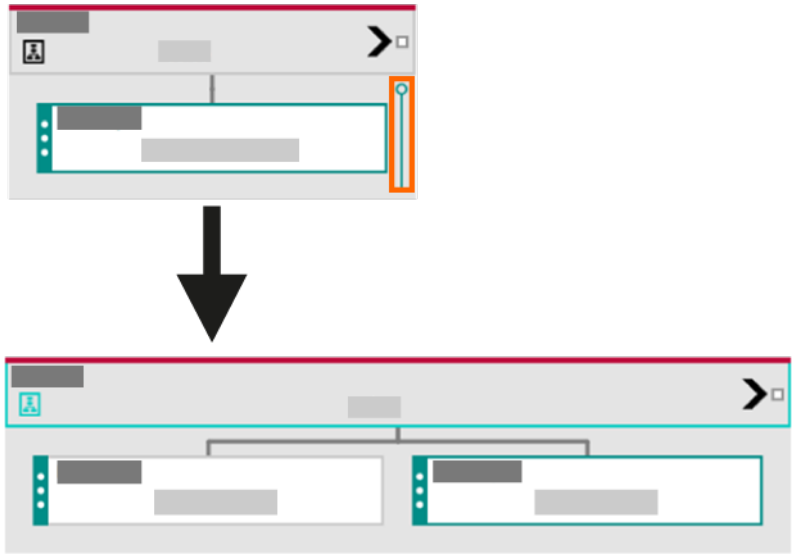
- Click on to open the **Library** window.
- Use drag and drop to insert the desired commands into the method in **Library** ▶ **Commands**.

Commands can be inserted either one below the other or side by side:

- Commands that are aligned one below the other are executed **sequentially**. A green horizontal line shows the insertion position of a command.



Commands that are aligned side by side are executed in **parallel**. A green vertical line shows the insertion position of a command.



The following options are available for inserting and editing commands and methods:

- Commands can be moved within the method using drag and drop or they can be deleted from the method by clicking on ✕ or **[Delete]**.
- Device-dependent commands can be inserted only into methods, but not into operating procedures.
- Commands can be copied from operating procedures or methods with **[CTRL]**+**[C]** and inserted in other operating procedures or methods with **[CTRL]**+**[V]**. Commands cannot be copied within the run of the commands **LOOP**, **IF** and **SEQUENCE**.
- Methods cannot be edited in the operating procedures editor. In order to edit it, the method must be opened in the method editor.
- Methods can be inserted repeatedly in an operating procedure.

6 Naming or renaming a command

- Select the desired command.
- Click on to open the **Properties** window.
- Enter the desired name in the **Name** field under **Properties** ▶ **General**.

7 Entering a comment (optional)

- Enter the desired comment in the **Comment** field under **Properties** ▶ **General**.

A command containing a Comment is indicated with in the method editor and operating procedure editor.

8 Editing command parameters

- Select the desired command.
- Click on to open the **Properties** window.
- Change the desired command parameter in **Properties** ▶ **Parameters**.

9 Assigning functional units

- Select the desired command.
- Click on to open the **Properties** window.

- Activate the desired functional units in **Properties** ▶ **Execute with** which, in turn, assigns them to the command.

If the functional units can be uniquely assigned to the commands, this occurs automatically. If several functional units of the same type are available and no unique assignment is possible, then the functional units must be assigned manually.

10 Defining Solution conditions and Sensor conditions (optional)

Defining **Solution conditions** and **Sensor conditions** in accordance with the following instructions: *(see "Defining solution conditions and sensor conditions", chapter 5.12.7.4, page 1020)*

11 Inserting optional runs

- Click on to open the **Library** window.
- Use drag and drop to insert the desired optional run into the operating procedure in **Library** ▶ **Optional runs**.
- Insert the desired methods or commands in the optional run.

An optional run can be inserted only parallel to the standard run. Additional information on the optional runs:

(see "Run in case of a stop – Definition", chapter 5.11.6, page 428)

(see "Run in case of an error – Definition", chapter 5.11.5, page 427)

12 Validating a method manually (optional)

- Click on to start the method validation.

Metrohm recommends always validating the method before saving it so that any potential problems are identified immediately. If the validation is not successful, messages in the OMNIS Software will provide instructions for solving the problems.

Validation entails checking the assigned work systems (e.g. if a functional unit required for a command is missing, or if 2 functional units of the same type are present and assignment to the corresponding command must be carried out manually). The system checks whether the parameters lie within the valid input range. If a parameter lies outside of the input range, an error message is displayed when validating the method. With newly created methods starting with OMNIS Software Version 3.3.0, an additional check is made to determine whether there is a variable in the formula editor (e.g. command variable) that does not have a reference object (e.g. command name).

13 Saving the method

- Save the method by clicking on . The method is automatically validated during saving.

The method is saved. The version and change date of the method are updated automatically in **Properties** ▶ **General**.

In the **OMNIS Client/Server system**, a method can be published after saving it. Information on publishing methods: *(see "Publishing the operating procedure and the method", chapter 5.11.1.6, page 396)*

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Creating a work system (chapter 5.12.4.4, page 989)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Method – Definition (chapter 5.11.3, page 413)

Methods – Subsection (chapter 5.11.3.1, page 414)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Server method – Definition (chapter 5.11.4, page 425)

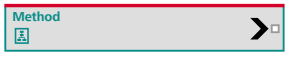
Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.3.4 Creating a method variable

Method-specific variables can be defined as **method variables**. These method variables are available in the operation procedures which contain this method. They are used for entering formulas in the formula editor in the **method variables** variable category, for instance in **CALC** commands.

1 Selecting the method and opening the properties

- Open the required method or create a new method under **Processes** ▶ **Methods** *(see "Creating and editing a method", chapter 5.11.3.3, page 418)*.

  Click on 

.
- Click on to open the **Properties** window.
  or
- Double-click on

to open the **Properties** window directly.

2 Adding a method variable

- In **Properties** ▶ **Parameters**, click on to add a new method variable.

To delete a method variable, right-click on an input field and select **[Delete input field]**.

3 Defining a method variable

- In the **Field name short** field, enter the name under which the method variable should be available in the formula editor.
- In the **Field name long** field, enter the name for the input field that should be used for designations in reports.
- In the **Type of input field** field, select the desired type (**Text** or **Number**) for the information.
- In the **Default value** field, enter the desired default value for the variable.

The variable defined in the method is displayed in the formula editor, for instance for **CALC** commands.

4 Saving a method

- Save the method by clicking on .

The method is saved. The version and change date of the method are updated automatically in **Properties** ▶ **General**.

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Creating a work system (chapter 5.12.4.4, page 989)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

5.11.4 Server method – Definition

A **Server method** is understood to be an method that is located on the OMNIS Server and is thus available to all connected OMNIS Clients.

A server method defines a combination of commands that can be aligned sequentially and in parallel.

Prerequisite for the use of a server method:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The server method has already been downloaded and is available under **Processes** ▶ **Methods**. The associated work systems, models, model hierarchies slope/y-intercept corrections, solution conditions, and sensor conditions are also downloaded when a server method is downloaded and listed in the corresponding subsections.

A server method can be downloaded under **Processes** ▶ **Server methods** by clicking on .
When downloading a subsample from a server search query, the associated server methods are automatically downloaded.

- The server method must be contained in an **operating procedure**.
- At least one **work system** is assigned to the server method.

After downloading, all functional units of the published work system must be replaced by functional units from custom devices via drag-and-drop and the work system must be saved. No additional functional units can be added to a published work system, nor can any functional units be removed from it.

There is no limit to the number of times saved server methods can be used in various operating procedures at the same time.

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Server methods – Subsection (chapter 5.11.4.1, page 426)

Server operating procedure – Definition (chapter 5.11.2, page 410)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.4.1 Server methods – Subsection

The following functions are available under **Processes** ▶ **Server methods**:

- **Download methods** downloads the selected methods and the associated work systems, models, model hierarchies, slope/y-intercept corrections, solution conditions, and sensor conditions. The downloaded methods and the associated work systems, models, model hierarchies and slope/y-intercept corrections, solution conditions and sensor conditions are listed in the corresponding subsections and can be used.
- **Update view** updates the list of the server methods. All entries are reloaded.
- Use **Delete server methods** to delete all selected server methods. To be able to delete the server methods, these must first be withdrawn. The deleted methods are retained locally in the status **withdrawn** on the OMNIS Clients which downloaded the server methods before they were deleted.

Server methods can be filtered by names and tags. Additional information on filtering server methods: *(see "Filtering tags", chapter 5.9.2, page 206)*

Overview list

The following information is displayed in the overview list:

Name	Name of the server method.
Published	Status of the server method. Additional information: *(see "Operating procedures and methods – Status", chapter 5.11.1.8, page 401)*
Saved	Time at which the server method was last saved.
Version	Version number of the server method. A server method always has the version number 1.
Tags	Existing tags assigned to this server method.
Data permissions	Existing data permissions assigned to this server method. **Note**: Applies only if data permissions are enabled and the user has the necessary user rights.

See also

Data permissions – Definition (chapter 4.5.9, page 105)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operating procedures and methods – Status (chapter 5.11.1.8, page 401)

Publishing the operating procedure and the method (chapter 5.11.1.6, page 396)

Server method – Definition (chapter 5.11.4, page 425)

Server operating procedures – Subsection (chapter 5.11.2.1, page 412)

Withdrawing operating procedure and method (chapter 5.11.1.7, page 400)

5.11.5 Run in case of an error – Definition

The optional **Execute on error** run can be inserted into a **Method** or **Operating procedure**. If this run sequence is included in a method, then **Commands** can be inserted. If this run sequence is included in an operating procedure, then **Methods** and **Commands** can be inserted. These are executed in the event of an error. This makes it possible, for instance, to switch off running pumps or move the robot arm to the park position in case of an error.

Optional runs can only be inserted parallel to the run of a method or an operating procedure. Sequential and parallel sequences of commands and methods can be reproduced in the optional runs.

If an error occurs during a determination that leads to cancellation of the determination, the corresponding runs of the **Execute on error** type for all methods which have already been completed or started will be executed. These run sequences are executed in the same order as the methods in the run. The functional units of the same work system used for executing the method are used for the commands in the run sequences.

It is not until after the end of the optional sequences of all methods which have been completed or started that the **Execute on error**-type run is executed on the level of the operating procedure.

If an error occurs or a stop is triggered manually when executing an **Execute on error**-type run, then the run will be canceled immediately.

See also

Method – Definition (chapter 5.11.3, page 413)

Operating procedure – Definition (chapter 5.11.1, page 379)

Run in case of a stop – Definition (chapter 5.11.6, page 428)

5.11.6 Run in case of a stop – Definition

The optional **Execute on stop** run can be inserted into a **Method** or **Operating procedure**. If this run sequence is included in a method, then **Commands** can be inserted. If this run sequence is included in an operating procedure, then **Methods** and **Commands** can be inserted. These are executed in the event of a manually triggered stop. This makes it possible, for instance, to switch off running pumps or move the robot arm to the park position in case of a stop.

Optional runs can only be inserted parallel to the run of a method or an operating procedure. Sequential and parallel sequences of commands and methods can be reproduced in the optional runs.

If a stop is triggered manually during a determination, the corresponding **Execute on stop**-type runs of all methods which have already been completed or started will be executed. These run sequences are executed in the same order as the methods in the run. The functional units of the same work system used for executing the method are used for the commands in the run sequences.

It is not until after the end of the optional runs of all methods which have been started or completed that the **Execute on stop** run is executed on the level of the operating procedure.

If an error occurs during the execution of an **Execute on stop** run, then the **Execute on error** run is executed for all methods which have already been completed or started.
If the stop button is pressed during the execution of an **Execute on stop**-type run, then the run is stopped.

See also

Method – Definition (chapter 5.11.3, page 413)

Operating procedure – Definition (chapter 5.11.1, page 379)

Run in case of an error – Definition (chapter 5.11.5, page 427)

5.11.7 Run in case of a limit value violation – Definition

The optional **Execute on limit** run can be inserted into an **Operating procedure**. **Commands** and **Methods** that should be executed in case of a limit value violation can be inserted into this run sequence.

Optional runs can only be inserted in parallel to the run of an operating procedure. Sequential and parallel sequences of commands and methods can be reproduced in the optional runs.

If a limit value violation occurs during a determination with result monitoring or for a control chart, then the corresponding **Execute on limit** run will be executed. The functional units of the same work system are used for the methods in the run sequence that was used when executing the method.

As many optional runs **Execute on limit** can be inserted into an operating procedure as needed.

All optional **Execute on limit** runs defined in the operating procedure are listed in the **Action** selection list in **Result monitoring** or during the creation or editing of a **Control chart**.

See also

NOTIFY – Parameters (chapter 5.11.8.72, page 787)

Operating procedure – Definition (chapter 5.11.1, page 379)

Recording the result monitoring (chapter 5.11.1.11.1, page 408)

Result monitoring – Definition (chapter 5.11.1.11, page 408)

5.11.8 Commands – Definition

Commands are used to create methods or operating procedures. Commands have the following properties:

- **Command type**
  The command type defines the function of the command. The designation of the command type is language-neutral (i.e. the designation or abbreviated designation is in English for all languages) and cannot be changed.
- **Command name**
  Each command has a freely selectable command name that is entered under **Processes** ▶ **Method** ▶ **Command** in the **Properties** window: *(see "Command – Properties", chapter 5.11.8.1, page 431)*
- **Comment**
  A Comment can be added to each command in the **Properties** window under **Processes** ▶ **Method** ▶ **Command**.

Appearance

Commands are displayed in two-line format. The first line contains the name of the command type (e.g. **DET pH**, **CALC**) and the second line contains a freely selectable command name.

The left-hand edge of the command element is color-coded for the various types of commands:

-
  Measuring commands, calibration commands and titration commands
-
  Structure commands that control the process sequence (e.g. branches and loops)
-
  Dosing commands, automation commands and other commands

Commands that contain a Comment are identified with .

Command variables

Each command has at least one command variable that is created in the process sequence and can be used under the '**Variable name**.*Command name*' designation.

The following variable is available for all commands:

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

All the commands that have more than one variable are featured in a separate topic that contains information on their variables.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

Method – Definition (chapter 5.11.3, page 413)

Operating procedure – Definition (chapter 5.11.1, page 379)

5.11.8.1 Command – Properties

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 3 subsections **General**, **Parameters** and **Execute with**:

General

Name	Enter the command name (editable, max. 255 characters). If a command is renamed afterwards, the cross-references to this command (e.g. command variables) are adjusted automatically within the operating procedure and methods. **Note:** Under certain circumstances, the references cannot be adjusted automatically. In this case, when saving a method or operating procedure and during method validation , a message appears with notes on how to solve the problem. The saving process will not be blocked, despite these messages. The validation is applied only to operating procedures and methods that have been created starting with OMNIS Software version 3.3.0.
Object ID	Display the identification number of the command.
Comment	Comment on the command (can be edited, max. 255 characters).

Parameters

In this subsection, depending on the command, various different parameters are available that can be adjusted individually. For certain commands, e.g. dosing commands, it is necessary to observe the information in the **Properties** of the functional unit.

For some functional units or auxiliary equipment there is a variety of data available in the properties of the overview of the instrument and in the specific subsections (e.g. sample racks or sensors).

Execute with

A work system with appropriate functional units must be assigned to the method that contains the command beforehand. Then the functional units in the work system are assigned to individual commands automatically if the required functional units are available in the work system and these functional units can be uniquely assigned. If several functional units of the same type are available, then the system is not able to uniquely assign the functional unit. In such cases, the desired functional unit has to be assigned to the command manually.

Further information on assigning functional units: *(see "Assigning a functional unit to a command", chapter 5.12.3.3, page 905)*

In this subsection, it is possible to define the **Solution conditions** and the **Sensor conditions**, depending on the command and the functional unit.

Additional information for defining solution conditions and sensor conditions: *(see "Defining solution conditions and sensor conditions", chapter 5.12.7.4, page 1020)*

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Assigning a work system to a method (chapter 5.12.4.5, page 990)

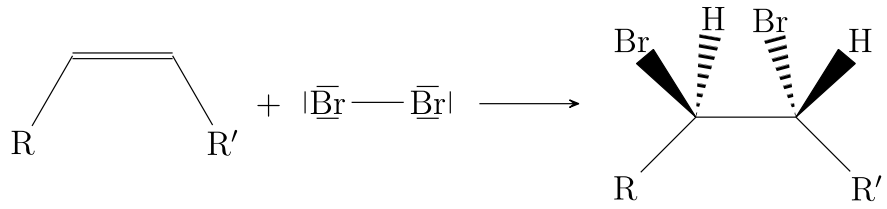
Creating and editing a method (chapter 5.11.3.3, page 418)

Variables – Directory (chapter 5.11.9.3, page 827)

5.11.8.2 Coulometric bromine index determination – Principle

The bromine index is a key figure for the proportion of unsaturated hydrocarbons in various mineral oil products. It defines the amount of bromine consumed by 100 g of sample under the given conditions. The bromine index is an important quality control parameter for mineral oil products.

The analytical process consists of adding a defined amount of bromine to the sample, whereby the bromine is chemically added to the carbon-carbon double bond.



Principle of the coulometric bromine index determination

In the coulometric bromine index determination, the constant current applied to the generator electrode between the anode and cathode releases the stoichiometrically corresponding amount of bromine from the bromide-containing reagent by electrolysis. The bromide contained in the reagent is oxidized to bromine at the anode, while hydrogen ions are reduced to hydrogen at the cathode. The endpoint of the titration is detected with an indicator electrode (polarizable metal electrode: Double Pt electrode).

As soon as bromine is present in excess, i.e. no more bromine is consumed by the sample, a reversible bromine-bromide redox system will be formed. In the case of a coulometric bromine index determination with voltametric measurement, this leads to a voltage drop at the indicator electrode. The current-time area for bromine generation is determined during titration. The amount of bromine produced is calculated from this.

The coulometric bromine index determination can be carried out in 2 different ways:

- With a discontinuous controller (2-point controller), resulting in a 2-phase cycle: "Generator on" and "Generator off" (according to ASTM D1492; CC = Continuous Current)
- With a continuous controller that generates a continuously controlled current at the generator electrode (PC = Pulsed Current, as with the 851/852 Titrando).

The principle of coulometric titration according to ASTM D1492 is described below. According to the standard, this method is suitable for samples with a bromine index of up to 100.

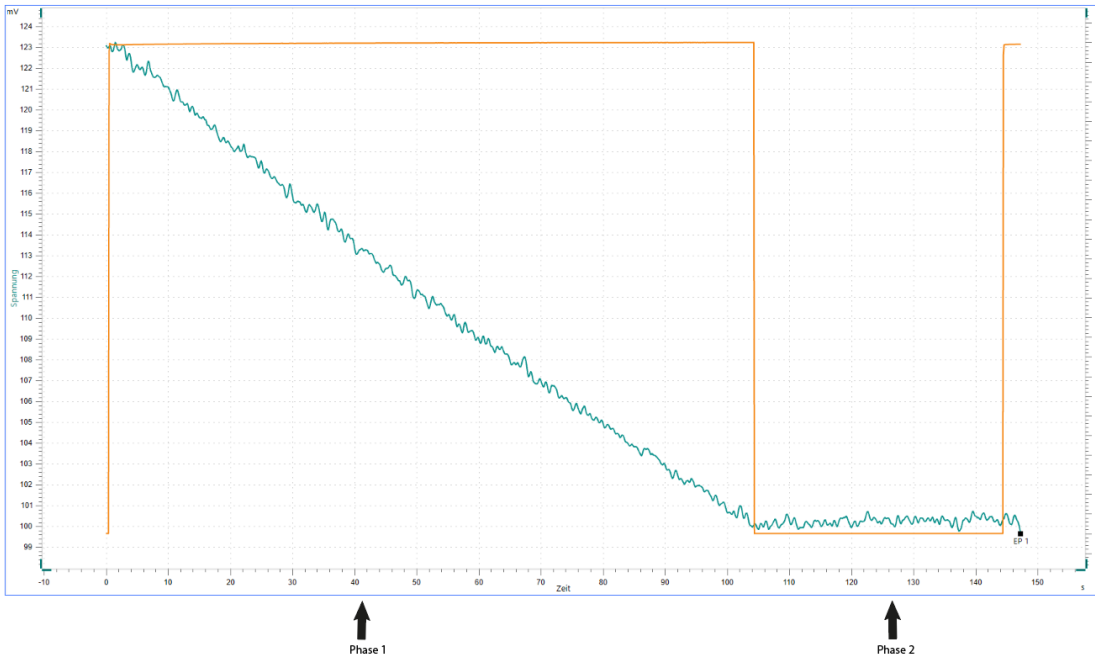
The measuring signal must be close to the endpoint before titration. This is achieved by pretitration. For this purpose, Metrohm recommends a small sample addition before the first analysis.

2-phase cycle

In contrast to the coulometric Karl Fischer titration, in which the generation of iodine is driven by continuous regulation of the generator current so that the predefined endpoint is reached as quickly and accurately as possible, in the coulometric bromine index determination according to ASTM D1492, the endpoint can be reached immediately or by repeating the 2-phase cycle to reach the end of titration.

- **Phase 1**: The generator is operated with a defined fixed generator current until the endpoint is reached. If the endpoint is reached in less than a defined time (parameter **Minimum generator on time**; according to the above-mentioned standard: 4 s), the titration is considered to have been completed in regular fashion.
- **Phase 2**: If it takes longer than the defined minimum generator on time to reach the endpoint, then the generator is switched off for a defined time after reaching the endpoint (parameter **Generator off time**; according to the above-mentioned standard, this time is approximately 40 s). The new cycle then begins with phase 1.

The total consumption of bromine is required to calculate the bromine index. This results from the sum of the measured bromine consumption of all phases 1.



See also

BRC CC Ipol – Command variables (chapter 5.11.8.2.3, page 441)

BRC CC Ipol – Properties (chapter 5.11.8.2.1, page 435)

Coulometric bromine index determination – Sequence (chapter 5.11.8.2.2, page 439)

5.11.8.2.1 BRC CC Ipol – Properties

The **BRC CC Ipol** command is a titration command for coulometric bromine index determination, based on the ASTM D1492 standard. The coulometric bromine index determination is used for determination of unsaturated hydrocarbons in a wide variety of mineral oils in order to assess their quality.

After selecting the **BRC CC Ipol** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **BRC CC Ipol** command:

Parameters

Start conditions	
Signal drift initial measured value	The initial measured value is applied as soon as the signal drift falls below the defined value or no later than after the maximum waiting time has expired. **Off** deactivates the drift control.
Minimum waiting time	If drift control is activated, then the initial measured value will not be applied until after the minimum waiting time has expired at the earliest, even if it has already fallen below the **Signal drift initial measured value**.
Maximum waiting time	The initial measured value is adopted after the maximum waiting time has expired.
Pause	Waiting time before the start of the recording of the titration curve.

Endpoint control parameters	
Measuring mode	Type of generation of the polarization current. ▪ **Alternating current (AC)**: The polarization current is generated with alternating current (default value). ▪ **Direct current (DC)**: The polarization current is generated with direct current.
Polarization current	The current that is applied to the indicator electrode during voltametric measurement. The polarization current depends on the measuring mode. Predefined values can be selected when selecting **Alternating current (AC)**. The value can be freely defined when selecting **Direct current (DC)**.
Endpoint at	Measured value for the endpoint. The default value 100.0 mV with a polarization current **I(pol) AC** of 10 µA and the default value of 200.0 mV with a polarization current **I(pol) DC** of 1.0 µA is valid for most applications.

Endpoint control parameters	
Generator current	Polarization current that is applied at the generator electrode to generate bromine. According to the standard, the value should be defined as 5.0 mA (default value) or 1.0 mA.
Generator off time	Time during which the generator is switched off. The default value is 40 s according to the standard. Once this time has elapsed, the generator will be switched on again automatically.
Minimum generator on time	Minimum time, 4 s according to standard, during which the generator is switched on. The titration is stopped once the endpoint is reached within the minimum generator on time.

Titration parameters	
Extraction time	During the **Extraction time**, no endpoint is applied and the titration is not ended, even if the endpoint and the stop criterion have already been reached. The extraction time starts from the moment all start conditions have been processed. It is advisable to enter an **Extraction time**, e.g. for the titration of samples of low solubility.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The manually entered temperature is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the titration, even if the time interval has not yet been reached.
Carry out electrode check	▪ **Indicator electrode** (polarizable metal electrode): The electrode check is carried out at the start of the determination during the transition from an inactive normal status to titration. It checks within a few seconds whether an electrode is connected and whether a short circuit is present. ▪ **Generator electrode**: The electrode check is carried out during the determination as soon as current flows, i.e. in phase 1. The check verifies whether an electrode is connected and whether the resistance in the electrode is too high.

Stop conditions	
Stop time	The titration is canceled as soon as the defined time has elapsed since the start of the determination (including start conditions). **Off** disables this stop condition.
Fixed point evaluation	
Define fixed points	The subsection for defining the fixed points is opened. *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*
Specified quantity	Selection of the specified quantity for the calculation of the fixed point from the measuring point list: ▪ **Potential** The values **Time**, **Bromine** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Bromine** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Bromine** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified bromine content.
Fixed point at	Specified measured value for the calculation of the fixed point.
Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Bromine** ▪ **Potential** ▪ **Temperature** ▪ **Charge** ▪ **Ugen** ▪ **Igen**
Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Bromine** (default value) ▪ **Potential** ▪ **Temperature** ▪ **Charge** ▪ **Ugen** ▪ **Igen**

Chart – y2-axis	
Display y2-axis	If this option is activated, the second y-axis is shown for displaying another quantity as a curve.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Bromine** ▪ **Potential** (default value) ▪ **Temperature** ▪ **Charge** ▪ **Ugen** ▪ **Igen**

Curve simulation	
Curve selection	Simulated curves can be used with OMNIS instruments to check the determination run. The titration sequence is defined by the set parameters. The simulation must be deactivated before analyzing real samples. The following simulation curves can be selected: ▪ **None** (default value) No simulation curve (the curve simulation is deactivated). ▪ **Bromination (DC)** Titration curve for bromine index determination.

Additional information on the parameters (e.g., input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **BRC CC Ipol** command to be executed, the corresponding functional unit must be assigned to it:

Measuring Module Coulometry

The following parameters must also be defined:

Sensor name	Selection of the indicator electrode of the **Polarizable metal electrode** type that should be used at the **INPUT 1** measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the sensor of the **Temperature sensor** type that is to measure the temperature at the measuring input **INPUT 2** during the analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

BRC CC Ipol – Command variables (chapter 5.11.8.2.3, page 441)

Commands – Definition (chapter 5.11.8, page 429)

Coulometric bromine index determination – Principle (chapter 5.11.8.2, page 432)

Coulometric bromine index determination – Sequence (chapter 5.11.8.2.2, page 439)

Creating and editing a method (chapter 5.11.3.3, page 418)

KFC – Properties (chapter 5.11.8.11, page 586)

5.11.8.2.2 Coulometric bromine index determination – Sequence

A standard method for **BRC CC Ipol** may look as follows:

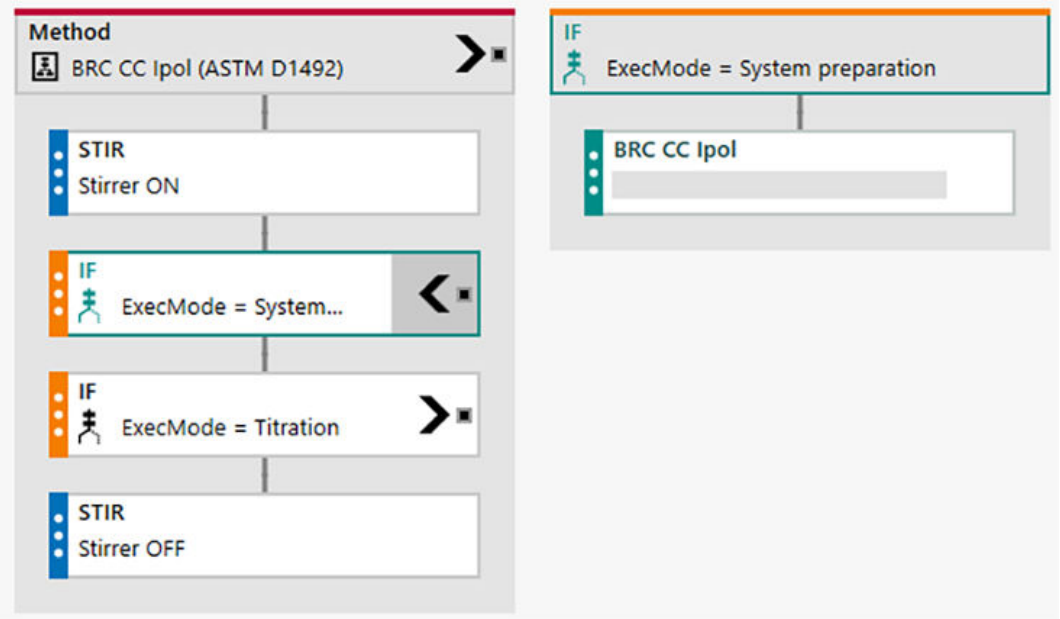


Figure 6 Preparing the system

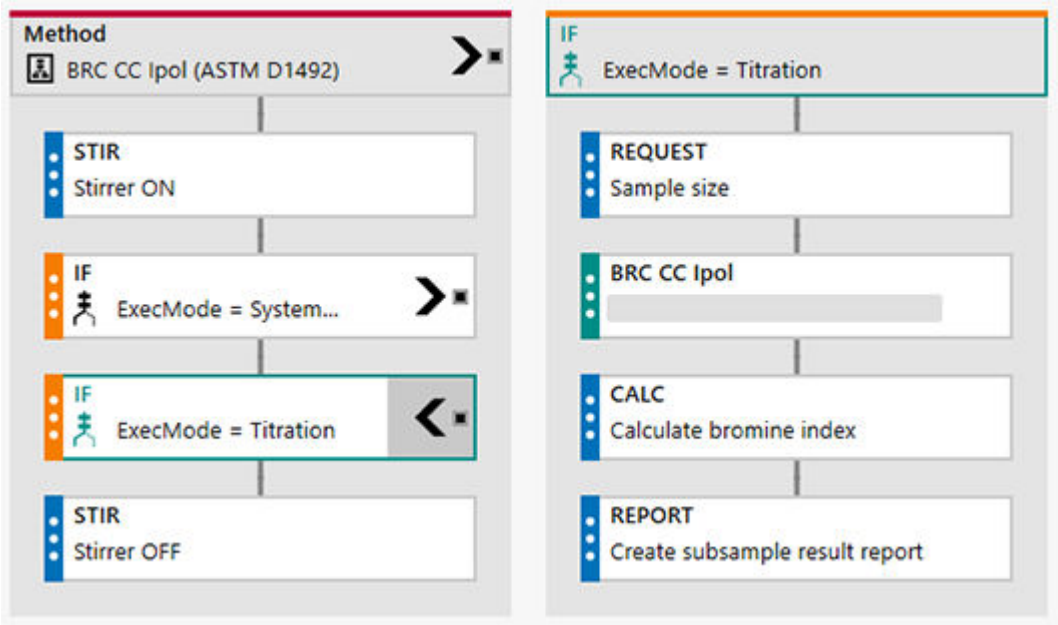


Figure 7 Titration

The **BRC CC Ipol** command is executed in the following steps:

1 – Preparing the system

The measuring signal must be close to the endpoint before titration. This is achieved by pretitration. For this purpose, Metrohm recommends a small sample addition before the first analysis.

2 – Processing the start conditions

The initial measured value (measured value before start of titration) is determined according to the parameters under **Start conditions**, either drift-controlled or after a maximum waiting time has elapsed. The defined **Pause** time is then observed.

3 – Carrying out the titration with the set control parameters and titration parameters

The titration is carried out according to the parameters defined under **Endpoint control parameters** and **Titration parameters**.

- **Fixed point evaluation**
  Optionally, up to 9 fixed points can be defined in **Fixed point evaluation** that are calculated from the measuring point list during the titration.
- **Chart – … axes**
  Quantities are predefined for the x-axis and the y-axis. However, other quantities can be selected. Optionally, **Display y2-axis** can be activated.

- **Curve simulation**
  Optionally, Curve simulation can be activated by selecting a simulation curve. This can be helpful for training purposes or for checking the method run without chemicals.
  During titration, the measured values are read out from the saved simulation curve.

No correct chemical titration is carried out with the Curve simulation setting.

4 – Exiting the titration

The titration is regularly completed as soon as the endpoint is reached in the same time or faster than defined in the **Minimum generator on time** parameter.

The condition defined under **Stop conditions** is constantly monitored during the titration.

A running titration can be canceled by a manual cancellation or with the emergency stop or in case of an error.

See also

BRC CC Ipol – Command variables (chapter 5.11.8.2.3, page 441)

BRC CC Ipol – Properties (chapter 5.11.8.2.1, page 435)

Coulometric bromine index determination – Principle (chapter 5.11.8.2, page 432)

KFC – Properties (chapter 5.11.8.11, page 586)

5.11.8.2.3 BRC CC Ipol – Command variables

The following variables are generated by the **BRC CC Ipol** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Amount.EP{1}**.*Command name*' Generated amount of bromine at the endpoint. Unit: µg
'**Amount.Final**.*Command name*' Generated amount of bromine after processing the command. Unit: µg

'**Amount.FP{1}**.*Command name*'

Generated amount of bromine at the fixed point.

Unit: µg

'**Charge.Final**.*Command name*'

Amount of charge for the last measuring point in the measuring point list.

Unit: mAs

'**Duration**.*Command name*'

Total duration for the processing of the command.

Unit: s

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**Index.EP{1}**.*Command name*'

Index of the endpoint.

Unit: None

'**Index.FP{1}**.*Command name*'

Index of the fixed point.

Unit: None

'**Measvalue.EP{1}**.*Command name*'

Measured value of the endpoint.

Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable

---

'**Measvalue.Final**.*Command name*'

End measured value after processing the command.

Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable

---

'**Measvalue.FP{1}**.*Command name*'

Measured value of the fixed point.

Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable

---

'**Temperature.EP{1}**.*Command name*'

Temperature associated with the endpoint.

Unit: °C

'**Temperature.Final**.*Command name*'

End temperature after processing the command.

Unit: °C

'**Temperature.FP{1}**.*Command name*'

Temperature associated with the fixed point.

Unit: °C

'**Time.EP{1}**.*Command name*'

Time stamp associated with the endpoint.

Unit: s

'**Time.Final**.*Command name*'

Time stamp for the last measuring point in the measuring point list.

Unit: s

'**Time.FP{1}**.*Command name*'

Time stamp associated with the fixed point.

Unit: s

'**Unit.Measvalue**.*Command name*'

Unit of the measured value.

Unit: mV

Equipment variables

'**Name.CurrentSensor**.*Command name*'

Name of the sensor used to measure the required measured quantity.

See also

BRC CC Ipol – Properties (chapter 5.11.8.2.1, page 435)

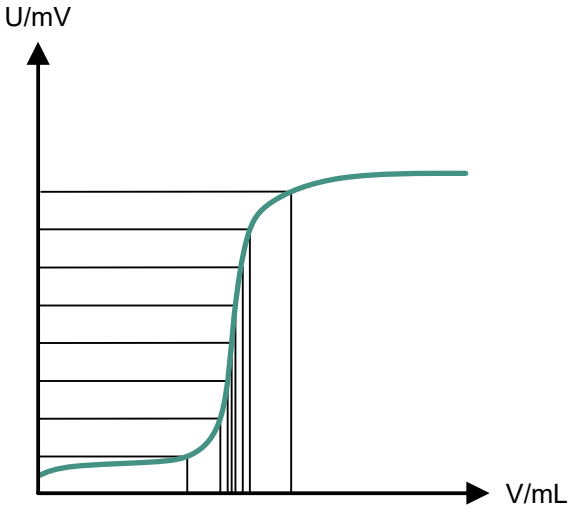
Coulometric bromine index determination – Principle (chapter 5.11.8.2, page 432)

Coulometric bromine index determination – Sequence (chapter 5.11.8.2.2, page 439)

5.11.8.3 DET – Principle

Measuring principle

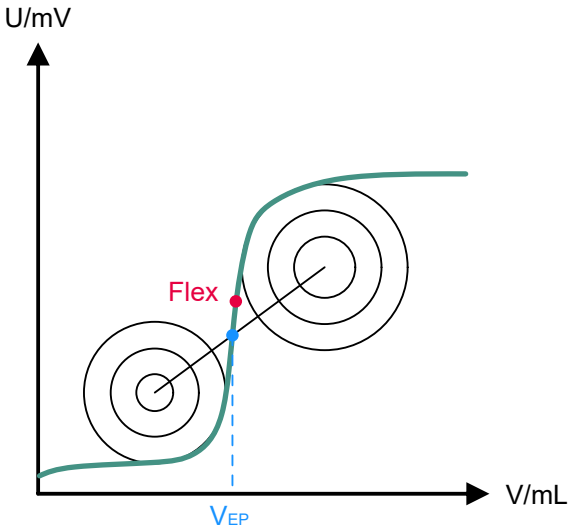
Titrations with dynamic reagent addition are carried out with the **DET** command. The volume increments are added in such a way, depending on the slope of the curve, that the measured value changes remain as constant as possible for each dosing. The optimal volume for dosing is determined from the measured value changes of the previous dosings. The measured values are applied either drift-controlled (equilibrium titration) or after a defined waiting time.



As the reagent dosing in **DET** depends on the measured data, the command parameters must be set so that the titration curve does not deviate too much from an s-shaped curve.

Potentiometric evaluation

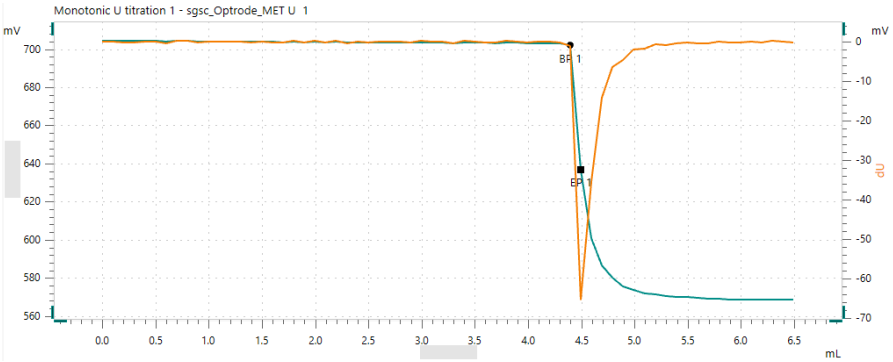
Equivalence points **EP** are evaluated automatically and are determined in a manner similar to that of the Tubbs method. With asymmetric titration curves, the volume value of the equivalence point $\mathbf{V_{EP}}$ is corrected by the inflection point **Flex** in the direction of the smaller circle of curvature.



The figure shows that the evaluation still requires measured values even after the equivalence point. The set EP criterion is compared to the calculated **ERC** (**E**quivalence point **R**ecognition **C**riterion) for the recognition of the equivalence points found. The ERC is the first derivative of the titration curve combined with a mathematical function that is more sensitive for flat jumps than for steeper ones. Equivalence points where the ERC is smaller than the set EP criterion will not be recognized.

Break point evaluation

A break point evaluation is used to determine sharp changes of direction in the titration curve. This evaluation is suitable for photometric titrations.



See also

Curves – Gran evaluation (chapter 5.10.11.4, page 328)

DET – Command variables (chapter 5.11.8.3.3, page 464)

DET – Properties (chapter 5.11.8.3.1, page 445)

5.11.8.3.1 DET – Properties

The **DET** command is used for executing dynamic equivalence point titrations (**DET** = **D**ynamic **E**quivalence Point **T**itration).

Depending on the measured quantity required, the following commands can be selected:

- **DET Ipol**
  Dynamic equivalence point titration with voltametric measurement with selectable polarization current (measured quantity: Potential U)
- **DET pH**
  Dynamic equivalence point titration with potentiometric pH measurement (measured quantity: pH)
- **DET U**
  Dynamic equivalence point titration with potentiometric potential measurement (measured quantity: Potential U)

The determination can be paused manually during the execution of a **DET** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped via the status menu.

After selecting a **DET** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions

and information are available for the commands **DET Ipol**, **DET pH** and **DET U**:

Parameters

Start conditions	
Signal drift initial measured value	The initial measured value is applied as soon as the signal drift falls below the defined value or no later than after the maximum waiting time has expired. **Off** deactivates the drift control.
Minimum waiting time	If drift control is enabled, the initial measured value will not be applied until after the minimum waiting time has expired at the earliest, and the measurement will be aborted, even if it has already fallen below the **Signal drift initial measured value**.
Maximum waiting time	**Drift control enabled:** If the signal drift does not fall below a defined value before the maximum waiting time has expired, then the initial measured value is adopted after the maximum waiting time has expired, and the measurement is aborted. **Drift control disabled:** The initial measured value is adopted after the maximum waiting time has expired and the measurement is canceled.
Start volume	The titrant is added before the start of titration until the start volume is reached. The following stop conditions are checked while dosing the start volume: ▪ **Stop volume** ▪ **Stop time**
Dosing rate start volume	Rate at which dosing takes place until the start volume has been reached. If, in the **Equipment** work area, a **Maximum dosing rate** is defined for dosing port 1 of the functional unit used that is smaller than the **Dosing rate start volume**, then the maximum dosing rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.

Start conditions	
Start measured value	The titrant is added before the start of titration until the start measured value is reached. The following stop conditions are checked while dosing the titrant: ▪ **Stop volume** ▪ **Stop measured value** ▪ **Stop time** **Off** disables this start condition. If the start measured value is already reached by dosing a start volume, then the start condition **Start measured value** is skipped. If the measured value does not change in this direction during dosing, then dosing is aborted without this start condition having been fulfilled.
Dosing rate start measured value	Rate at which dosing takes place until the start measured value has been reached. If, in the **Equipment** work area, a **Maximum dosing rate** is defined for dosing port 1 of the functional unit used that is smaller than the **Dosing rate start volume**, then the maximum dosing rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Start slope	The titrant is added until the start slope (measured value change per mL) is reached. The following stop conditions are checked while dosing the titrant: ▪ **Stop volume** ▪ **Stop measured value** ▪ **Stop time** **Off** disables this start condition.

Start conditions	
Dosing rate start slope	Rate at which dosing takes place until the start slope has been reached. If, in the **Equipment** work area, a **Maximum dosing rate** is defined for dosing port 1 of the functional unit used that is smaller than the **Dosing rate start volume**, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Pause	Waiting time, e.g. for the measured value to stabilize after start or as reaction time after dosing a start volume. The pause follows at the end of all the start conditions.

Titration parameters	
Titration rate	The titration rate can either be determined using 3 predefined parameter sets, or the values for the titration parameters can be defined individually. ▪ **Slow**: Parameter set for titrations for which the finest details are to be visible. This can, however, lead to an increase in noise, which may result in unwanted equivalence points. ▪ **Optimal**: Parameter set that has been optimized for the most common applications. ▪ **Fast**: Parameter set for not very critical, fast titrations. ▪ **Enter values**: The values for the titration parameters must be defined individually. If a predefined parameter set is selected for the titration rate, the following parameters are displayed but they cannot be edited: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** ▪ **Measuring point distance** ▪ **Minimum volume increment** ▪ **Maximum volume increment** ▪ **Dosing rate** The values used can be read in the corresponding parameters.
Signal drift	The measured value is adopted as soon as the signal drift falls below the defined value or no later than after the maximum waiting time has expired. Drift-controlled measured value acceptance is advisable if the time until a state of equilibrium is reached is variable. **Off** disables the drift control and the measured value is adopted after the maximum waiting time. A drift-controlled measured value acceptance is useful if the reaction runs slowly or if the electrode is slow to respond.

Titration parameters	
Minimum waiting time	If drift control is enabled, then the measured value will not be applied until after the minimum waiting time has expired at the earliest, even if it has already fallen below the **Signal drift**.
Maximum waiting time	**Drift control enabled:** If the signal drift does not fall below a defined value before the maximum waiting time has expired, the measured value is adopted after the maximum waiting time has expired. **Drift control disabled:** The measured value is adopted after the maximum waiting time has expired.
Measuring point distance	The smaller the measuring point distance, the smaller the volume increments and the slower the titration. The curve then reproduces all of the finest details, which, however, also means more noise and which could thus also lead to unwanted equivalence points being found. A small measuring point distance is particularly recommended for steep potential jumps (e.g. for strong acids or bases). The greater the selected measuring point distance, the larger the volume increments and the faster the titration. A greater measuring point distance is particularly recommended for flat potential jumps (e.g. for weak acids or bases). **Note**: This parameter is identical with the **measuring point density** parameter used in previous Metrohm applications. The numerical values can therefore be applied 1:1.
Minimum volume increment	Minimum permitted volume increment that is dosed at the start of the titration and in the event of steep potential jumps in the region of the equivalence point. A small value (< 10 µL) is only advisable if very low titrant consumption is expected (e.g. EP volume < 0.5 mL). Otherwise, unwanted equivalence points may appear.

Titration parameters	
Maximum volume increment	Maximum permitted volume increment that may be added per dosing step. The value for the maximum volume increment should not be less than 1/100 of the cylinder volume. With **Unlimited**, the maximum possible volume increment will not be restricted. The maximum volume increment should be limited in the following cases: ▪ The titrant consumption is very low until the equivalence point is reached. ▪ A start volume is dosed until shortly before the equivalence point is reached. ▪ The change of direction in the jumping range is very abrupt, because otherwise it is easily possible for an excessively large volume to be dosed in the range of the equivalence point. **Note:** Avoid similar values for the **Minimum volume increment** and **Maximum volume increment** parameters. Monotonic equivalence point titration (MET) is more appropriate for such applications.
Dosing rate	Rate at which the volume increments are dosed. If a smaller **Maximum dosing rate** is defined for dosing port 1 of the used functional unit in the **Equipment** work area, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The input field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected.

Titration parameters	
I(pol) DC (only for DET Ipol)	The polarization current **I(pol) DC** (Direct Current) is the current that is applied to the polarizable electrode during voltametric measurement. **Note**: For OMNIS instruments, Metrohm recommends entering the current in increments of 0.5 µA. For instruments of the **Titrando** type an increment of 0.5 µA **must** be observed. For instruments of the **855 Robotic Titrosampler** type an increment of 2.5 µA **must** be observed.
Carry out electrode check (only for DET Ipol)	The electrode check is carried out for polarizable electrodes during the transition from an inactive normal status to the titration. It checks within a few seconds whether an electrode is connected and whether no short circuit is present.
Filling rate	Rate at which the cylinder is filled. If, in the **Equipment** work area, a smaller **Maximum filling rate** is defined for the fill port for the functional unit used, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if air bubbles form during the aspiration of the solution, then the filling rate must be reduced accordingly so that the dosing drive is not overloaded.
Stop conditions	
Stop volume	The titration is canceled as soon as the defined volume has been dosed since the start of the titration (including start conditions). The volume must be adjusted to the size of the titration vessel to prevent it from overflowing. In addition, the **Stop volume** should always be smaller than or equal to the cylinder volume to avoid refilling during the titration. **Off** disables this stop condition.
Stop measured value	The titration is canceled as soon as it falls below or exceeds the defined measured value since the start of the titration. Exceeding or falling below the stop measured value is monitored on the basis of the titration direction which is defined internally using the stop measured value and the start measured value (or the initial measured value if the start measured value is disabled). **Off** disables this stop condition.
Stop EP	The titration is aborted as soon as the specified number of equivalence points (EP) has been evaluated according to the **EP criterion** parameter. **Off** disables this stop condition.

Stop conditions	
Volume after EP	As soon as the number of equivalence points defined under **Stop EP** has been evaluated, the **Volume after EP** is added to the volume of the last equivalence point. The titration is canceled after this total volume has been dosed. Because determination of the equivalence point requires titration in excess of the equivalence point, the end volume will be greater than the equivalence point volume that leads to the action being canceled, even if **Volume after EP** = 0 mL. **Note**: This parameter was deactivated in previous Metrohm applications with **Off**, which now corresponds to the setting "0 mL".
Stop time	The titration is canceled as soon as the defined time has elapsed since the start of the determination (including start conditions). **Off** disables this stop condition.

Potentiometric evaluation	
Selection of the type	Selection whether the equivalence points are evaluated and recognized throughout the entire titration curve (**Regular**) or only in certain segments of the curve (**Window-based**). The fields **EP criterion** and **EP recognition** only appear in the **Regular** setting. If **Window-based** is selected, then multiple evaluation windows can be defined or edited: *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*.
EP criterion	Threshold value for the evaluation of equivalence points. Equivalence points are not evaluated if the calculated **ERC** value (ERC = **E**quivalence point **R**ecognition **C**riterion) is smaller than the defined value.
EP recognition	Filters for the recognition of equivalence points: ▪ **All** All evaluated equivalence points are recognized. ▪ **Last** Of the evaluated equivalence points, only the last is recognized. ▪ **Greatest** Of the evaluated equivalence points, only the one with the greatest ERC value (i.e. with the steepest curve section) is recognized. ▪ **Off** The evaluation and recognition of equivalence points is switched off.
[Edit evaluation windows]	The window for defining the evaluation windows is opened. *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*

Fixed point evaluation	
Define fixed points	The window for defining the fixed points is opened. *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*
Specified quantity	Selection of the specified quantity for the evaluation of the fixed point from the measuring point list: Only valid for **DET Ipol**: ▪ **Potential** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume. Only valid for **DET pH**: ▪ **pH** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified pH value. ▪ **Time** The values **pH**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **pH**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume. Only valid for **DET U**: ▪ **Potential** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume.
Fixed point at	Specified measured value for the evaluation of the fixed point.

Break point evaluation	
Selection of the type	Selection whether the break points are evaluated throughout the entire titration curve (**Regular**) or only in certain segments of the curve (**Window-based**) or not at all (**Off**). If **Window-based** is selected, then multiple evaluation windows can be defined or edited: *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*.

Break point evaluation	
BP criterion	Criterion for the evaluation of break points. Standardized difference between maximum and minimum of the second derivative. Break points with a found **BRC** value (BRC = **B**reakpoint **R**ecognition **C**riterion) that is smaller than the value entered here will not be evaluated.
Min. deflection	Threshold value of the slope difference between the sections before and after the break point. The smaller the difference, the more break points will be evaluated.
Max. expected BPs	Maximum number of break points that are expected. The curve is smoothed until the number of evaluated break points is smaller or equal to this number.
BP recognition	Filters for the recognition of break points: ▪ **All** All evaluated break points are recognized. ▪ **First** Of the evaluated break points, only the first one is recognized. ▪ **Last** Of the evaluated break points, only the last one is recognized.
[Edit evaluation windows]	The window for defining the evaluation windows is opened. *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*

Gran evaluation	
Selection of the type	Selection as to whether the titration curve is evaluated according to the Gran procedure (**Gran point**) or not (**Off**). If **Gran point** is selected, then a Gran point is determined for the titration.
Reaction type	Selection of the reaction type (analyte, titrant). The available options for the parameter **Gran plot** are displayed, depending on the selection. ▪ **Weak monoprotic acid, strong base**: Titration of a weak monoprotic acid with a strong base. ▪ **Weak monoprotic base, strong acid**: Titration of a weak monoprotic base with a strong acid. ▪ **Strong base, strong acid or strong acid, strong base**: Titration of a strong base with a strong acid or a strong acid with a strong base.

Gran evaluation	
Gran plot	Range of the titration curve that is used to determine the Gran point. Specifying the lower limit and the upper limit for the selected segment makes it possible to define the linear range in which the measuring points for the determination of the regression line are used. Depending on the selection of the reaction type, the parameters for the Gran function used for the evaluation can also be defined. ▪ **Acidic segment**: If the analyte is acidic, then the segment is used before the equivalence point. If the analyte is alkaline, then the segment after the equivalence point is used. If **Acidic segment** is selected, the following specific parameters appear: – **Initial volume** (does not apply for Weak monoprotic acid, strong base) – **Lower limit pH acidic** – **Upper limit pH acidic** ▪ **Alkaline segment**: If the analyte is acidic, then the segment after the equivalence point is used. If the analyte is alkaline, then the segment before the equivalence point is used. If **Alkaline segment** is selected, the following specific parameters appear: – **Initial volume** (does not apply for Weak monoprotic base, strong acid) – **Lower limit pH alkaline** – **Upper limit pH alkaline** ▪ **Acidic and alkaline segment**: Not only the segment before the equivalence point but also the segment after the equivalence point are both used. If **Acidic and alkaline segment** is selected, the following specific parameters appear: – **Initial volume** – **Lower limit pH acidic** – **Upper limit pH acidic** – **Lower limit pH alkaline** – **Upper limit pH alkaline** **Note:** The **Lower limit pH** and the **Upper limit pH** must be defined for each segment in such a way that both limits are located on the same side of the equivalence point. ▪ **Normalized**: The entire titration curve is used. The standardized procedure is available only for the reaction type **Strong base, strong acid or strong acid, strong base**. If **Normalized** is selected, the following specific parameters appear: – **Initial volume** – **Lower limit pH** – **Upper limit pH** **Note:** The selection **Normalized** corresponds to the evaluation procedure in previous Metrohm applications. Additional information regarding the Gran functions applied: *(see "Curves – Gran evaluation", chapter 5.10.11.4, page 328)*

Gran evaluation	
Initial volume	Volume of the analyte that is in the sample vessel before the titration is started.
Lower limit pH acidic, **Lower limit pH alkaline** or **Lower limit pH**	Defines the lower limit of the range in which the measuring points for determining the regression line are used.
Upper limit pH acidic, **Upper limit pH alkaline** or **Upper limit pH**	Defines the upper limit of the range in which the measuring points for determining the regression line are used.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: Only valid for **DET Ipol**: ▪ **Potential** Only valid for **DET pH**: ▪ **pH** ▪ **Gran function value** If **Gran function value** is selected, the following specific parameter appears: – **Displaying regression lines** Only valid for **DET U**: ▪ **Potential** Valid for all commands: ▪ **Volume** (default value) ▪ **ERC** ▪ **Time** ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: Only valid for **DET Ipol**: ▪ **Potential** (default value) Only valid for **DET pH**: ▪ **pH** (default value) ▪ **Gran function value** If **Gran function value** is selected, the following specific parameter appears: – **Displaying regression lines** Only valid for **DET U**: ▪ **Potential** (default value) Valid for all commands: ▪ **Volume** ▪ **ERC** ▪ **Time** ▪ **Temperature**
Displaying regression lines	Display of at least one regression line that runs through the values of the selected quantity. The check box is used for activation. The regression lines are displayed only if the quantity **Gran function value** is selected for the corresponding y-axis or y2-axis and the quantity **Volume** is selected for the x-axis. The display is disabled by default. In addition, the Gran function values used for the calculation of the regression lines are highlighted. The volume of the Gran point is shown as a vertical line.

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.

Chart – y2-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: Only valid for **DET Ipol**: ▪ **Potential** Only valid for **DET pH**: ▪ **pH** ▪ **Gran function value** If **Gran function value** is selected, the following specific parameter appears: – **Displaying regression lines** Only valid for **DET U**: ▪ **Potential** Valid for all commands: ▪ **Volume** ▪ **ERC** (default value) ▪ **Time** ▪ **Temperature**
Displaying regression lines	Display of at least one regression line that runs through the values of the selected quantity. The check box is used for activation. The regression lines are displayed only if the quantity **Gran function value** is selected for the corresponding y-axis or y2-axis and the quantity **Volume** is selected for the x-axis. The display is disabled by default. In addition, the Gran function values used for the calculation of the regression lines are highlighted. The volume of the Gran point is shown as a vertical line.

Curve simulation	
Curve selection	Simulated curves can be used with OMNIS instruments to check the determination run. The titration sequence is defined by the set parameters. The simulation must be deactivated before analyzing real samples. Selection of the simulation curve: ▪ **None** (default value) The curve simulation is disabled. ▪ **Hydrochloric acid** Simulation curve of the titration of hydrochloric acid with caustic soda (titration curve with one equivalence point). ▪ **Citric acid** Simulation curve of the titration of citric acid with caustic soda (titration curve with 3 equivalence points).

The curve simulation cannot be used for instruments of the **Titrando** and **855 Robotic Titrosampler** type.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift initial measured value**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Dosing rate start volume**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Start measured value**
  Minimum value: –1,200.0 mV
  Maximum value: 1,200.0 mV
- **Start measured value pH**
  Minimum value: –13.000
  Maximum value: 20.000
- **Dosing rate start measured value**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Dosing rate start slope**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Signal drift**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Dosing rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **I(pol) DC** (Titrando)
  Minimum value: –122.5 µA
  Maximum value: 122.5 µA
  Permitted increment: 0.5 µA
- **I(pol) DC** (855 Robotic Titrosampler)
  Minimum value: –122.5 µA
  Maximum value: 122.5 µA
  Permitted increment: 2.5 µA

- **Filling rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Stop measured value**
  Minimum value: –1,200.0 mV
  Maximum value: 1,200.0 mV
- **Stop measured value pH**
  Minimum value: –13.000
  Maximum value: 20.000
- **Fixed point at**
  Minimum value DET Ipol and DET U: –1,200.0 mV
  Maximum value DET Ipol and DET U: 1,200.0 mV
  Minimum value DET pH: –13.000
  Maximum value DET pH: 20.000

Execute with

In order for a **DET** command to be executed, the corresponding functional units and, for analog measuring inputs, the required sensor need to be assigned to the command.

- Dosing unit or buret to which the titrant is connected:
  Dosing Drive with connected **Cylinder Unit**, **800 Dosino** with connected **807 Dosing Unit**, **805 Dosimat** with connected **806 Exchange Unit** or **Internal Dosing Drive** with connected **806 Exchange Unit**
- Measuring input (digital or analog) to which the sensor required for the titration is connected:
  Measuring Module Digital, **Measuring Module Analog**, **Measuring Interface iConnect**, or **Measuring Interface Analog**
- Sensor (digital, intelligent or analog):
  Polarizable metal electrode, **Ion-selective electrode**, **pH electrode**, **Metal electrode** or **Other sensor**

After a functional unit for the command has been selected, the following additional parameters appear:

For **Dosing Drive**:	
Dosing port	Port that is to be used to dose a volume increment. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1 (default value). ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2.

For **Measuring Module Analog**:

Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input (only for DET pH and DET U)	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **Difference**: Differential measurement between electrodes at INPUT 1 and INPUT 2.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error. **Note**: For a combined pH/temperature sensor, both measuring inputs must be set to **INPUT 1**.
Measuring input (only for DET pH and DET U)	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.

For **Measuring Interface Analog** and **Measuring Interface iConnect** (DET pH and DET U):

Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **Ind./Ref./Temp.**: Measurement with an analog electrode. ▪ **iConnect**: Measurement with an intelligent electrode (iTrode)
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Measuring Interface Analog** (DET Ipol):	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: **Pol./Temp.**: Measurement with a polarizable electrode.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Curves – Fixed point evaluation (chapter 5.10.11.3, page 327)

Curves – Window-based evaluation (chapter 5.10.11.2, page 325)

DET – Command variables (chapter 5.11.8.3.3, page 464)

DET – Principle (chapter 5.11.8.3, page 443)

DET – Run (chapter 5.11.8.3.2, page 463)

KFC – Properties (chapter 5.11.8.11, page 586)

KFT – Properties (chapter 5.11.8.10.1, page 568)

MET – Properties (chapter 5.11.8.4.1, page 472)

SET – Properties (chapter 5.11.8.6.1, page 512)

Sensor – Definition (chapter 5.12.6, page 998)

5.11.8.3.2 DET – Run

The **DET** command is executed in 4 steps:

1 – Determining the initial measured value

The initial measured value (measured value before start of dosing) is determined according to the parameters in the parameter group **Start conditions**, either drift-controlled or after a maximum waiting time has elapsed.

2 – Processing the start conditions

If a **Start volume** was defined in **Start conditions**, it will be dosed before the actual titration.

The start conditions are checked in the following order: **Start volume ➔ Start measured value (pH) ➔ Start slope (pH)**

The defined **Pause** time is then observed.

3 – Carrying out the titration

The titration is carried out and evaluated according to the parameters defined under **Titration parameters** and **Potentiometric evaluation**.

- **Fixed point evaluation**
  Optionally, up to 9 fixed points can be defined in **Fixed point evaluation** that are calculated from the measuring point list during the titration.
- **Break point evaluation**
  The titration curve can be optionally evaluated according to the parameters defined under **Break point evaluation**.
- **Gran evaluation**
  The titration curve can be optionally evaluated according to the parameters defined under **Gran evaluation**.
- **Chart – … axes**
  Different quantities can be selected for the x-axis and y-axis. A y2-axis can be displayed as an option.

4 – Completing the titration

The titration is completed as usual as soon as the first stop condition defined in **Stop conditions** is reached.

A running titration can be canceled by a manual cancellation or with the emergency stop or in case of an error.

See also

DET – Command variables (chapter 5.11.8.3.3, page 464)

DET – Principle (chapter 5.11.8.3, page 443)

DET – Properties (chapter 5.11.8.3.1, page 445)

5.11.8.3.3 DET – Command variables

The following variables are generated by the commands **DET pH**, **DET U** and **DET Ipol** in the process sequence and can be used in a formula under the designation '**Variable name**.*Command name*'.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**ERC.EP{x}**.*Command name*' (x = 1–9) Calculated ERC value for the equivalence point. If this value is greater than or equal to the value defined in the **EP criterion** parameter, then the equivalence point will be recognized.
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**GranFunctionvalue.GP{x}**.*Command name*' (x = 1–9) Gran function value of the Gran point.
'**Index.BP{x}**.*Command name*' (x = 1–9) Index of the break point.
'**Index.EP{x}**.*Command name*' (x = 1–9) Index of the equivalence point.
'**Index.FP{x}**.*Command name*' (x = 1–9) Index of the fixed point.
'**Index.GP{x}**.*Command name*' (x = 1–9) Index of the Gran point.
'**InterceptAcidicSegment.GP{x}**.*Command name*' (x = 1–9) y-intercept of the regression line in the acidic segment of the Gran plot.

Command variables
'**InterceptAlkalineSegment.GP{x}**.*Command name*' (x = 1–9) y-intercept of the regression line in the alkaline segment of the Gran plot.
'**Measvalue.BP{x}**.*Command name*' (x = 1–9) Measured value of the break point. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.EP{x}**.*Command name*' (x = 1–9) Measured value of the equivalence point. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.FP{x}**.*Command name*' (x = 1–9) Measured value of the fixed point. Unit: None (DET pH) or mV (DET U, DET Ipol)
'**Measvalue.GP{x}**.*Command name*' (x = 1–9) Measured value of the Gran point.
'**NumberOfDataPointsAcidicSegment.GP{x}**.*Command name*' (x = 1–9) Number of Gran function values that are used to calculate the regression lines in the acidic segment of the Gran plot.
'**NumberOfDataPointsAlkalineSegment.GP{x}**.*Command name*' (x = 1 … 9) Number of Gran function values that are used to calculate the regression lines in the alkaline segment of the Gran plot.
'**SlopeAcidicSegment.GP{x}**.*Command name*' (x = 1–9) Slope of the regression line in the acidic segment of the Gran plot.
'**SlopeAlkalineSegment.GP{x}**.*Command name*' (x = 1–9) Slope of the regression line in the alkaline segment of the Gran plot.
'**SumOfSquaredErrorsAcidicSegment.GP{x}**.*Command name*' (x = 1 … 9) Sum of squares of the residuals, i.e. the deviation between the Gran function value and the corresponding point on the regression line, in the acidic segment of the Gran plot. The smaller the value, the better the regression line calculated by the regression analysis matches the corresponding segment of the Gran plot. The standard deviation can be calculated from the error sum of squares and the number of Gran function values considered for the regression line.

Command variables
'**SumOfSquaredErrorsAlkalineSegment.GP{x}**.*Command name*' (x = 1 … 9) Sum of squares of the residuals, i.e. the deviation between the Gran function value and the corresponding point on the regression line, in the alkaline segment of the Gran plot. The smaller the value, the better the regression line calculated by the regression analysis matches the corresponding segment of the Gran plot. The standard deviation can be calculated from the error sum of squares and the number of Gran function values considered for the regression line.
'**Temperature.BP{x}**.*Command name*' (x = 1–9) Temperature associated with the break point. Unit: °C
'**Temperature.EP{x}**.*Command name*' (x = 1–9) Temperature associated with the equivalence point. Unit: °C
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Temperature.FP{x}**.*Command name*' (x = 1–9) Temperature associated with the fixed point. Unit: °C
'**Temperature.GP{x}**.*Command name*' (x = 1–9) Temperature associated with the Gran point. Unit: °C
'**Time.BP{x}**.*Command name*' (x = 1–9) Time stamp associated with the break point. Unit: s
'**Time.EP{x}**.*Command name*' (x = 1–9) Time stamp associated with the equivalence point. Unit: s
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Time.FP{x}**.*Command name*' (x = 1–9) Time stamp associated with the fixed point. Unit: s

Command variables
'**Time.GP{x}**.*Command name*' (x = 1–9) Time stamp associated with the Gran point. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of measured values: None (DET pH) or mV (DET U, DET Ipol)
'**Volume.BP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the break point is reached. Unit: mL
'**Volume.EP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the equivalence point is reached. Unit: mL
'**Volume.Final**.*Command name*' End volume after processing the command, i.e. total dosed volume at the end of the command. Unit: mL
'**Volume.FP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the fixed point is reached. Unit: mL
'**Volume.GP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the Gran point is reached. Unit: mL

In the case of variables with index **{x}**, the index **{1}** is set automatically at the time of insertion in a formula. This index can be set manually to 2–9 (e.g., '**Volume.EP{3}**.*Command name*' for the volume of the third equivalence point).

Equipment variables
'**Concentration.CurrentSolution**.*Command name*' Concentration of the solution used that is dosed with the dosing unit or buret (corresponds to the concentration of component 1 in the solution used). Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable
'**Diameter.AspirationTube.CurrentSolution**.*Command name*' Diameter of the aspiration tubing that is connected to the Liquid Adapter. Unit: mm

Equipment variables
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the Liquid Adapter. Unit: cm
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.
'**Name.CurrentSolution**.*Command name*' Name of the solution used with the dosing unit.
'**Slope.CurrentSensor**.*Command name*' Quotient from the slope of the sensor used and the Nernst slope with the respective temperature. This variable is available only for pH electrodes. Unit: Determined by the sensor used.
'**Titer.CurrentSolution**.*Command name*' Titer of the solution connected to the Liquid Adapter that is dosed with the dosing unit. The titer is the factor that indicates the deviation of the actual concentration from the nominal concentration of a solution. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Concentration unit of the solution that is dosed with the dosing unit (corresponds to the concentration unit of component 1 in the solution). The unit is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer of the solution that is connected to the Liquid Adapter and that is dosed with the dosing unit.
'**ZeroPoint.CurrentSensor**.*Command name*' Electrode zero point of the sensor used. This variable is available only for pH electrodes. Unit: Determined by the sensor used.

See also

DET – Principle (chapter 5.11.8.3, page 443)

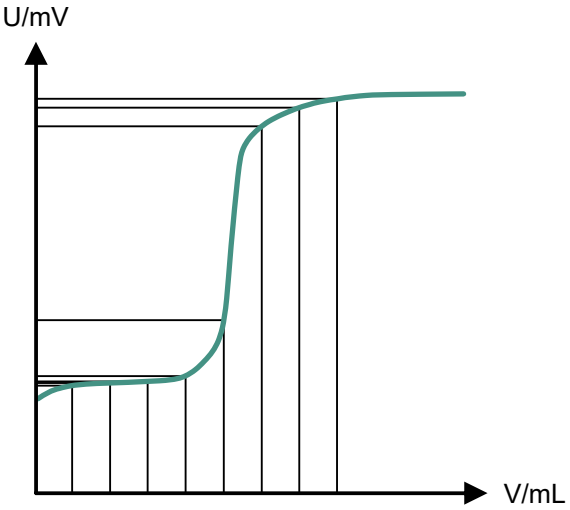
DET – Properties (chapter 5.11.8.3.1, page 445)

DET – Run (chapter 5.11.8.3.2, page 463)

5.11.8.4 MET – Principle

Measuring principle

Titrations with reagent addition at constant volume increments are carried out with the **MET** command. The measured values are applied either drift-controlled (equilibrium titration) or after a defined waiting time.



This command is suitable for titrations with relatively high signal fluctuations or suddenly occurring potential jumps and for slow titrations or electrodes which respond slowly.

Potentiometric evaluation (only MET pH, MET U, MET Ipol)

The equivalence points **EP** are automatically determined using a method based on the Fortuin method that has been adapted by Metrohm for numerical methods (for details, see *METROHM Bulletin, Vol. 2, No. 10, 1971*). Here, a search is carried out for the largest measured value change Δ_n. The exact **EP** is determined by using an interpolation factor ρ that depends on the Δ values before and after Δ_n:

$$V_{EP} = V_0 + \rho \, \Delta V$$

V_{EP} = EP volume, V_0 = total volume dosed before Δ_n, ΔV = volume increment, ρ = interpolation factor according to Fortuin

EP criterion in the MET command (only MET pH, MET U, MET Ipol)

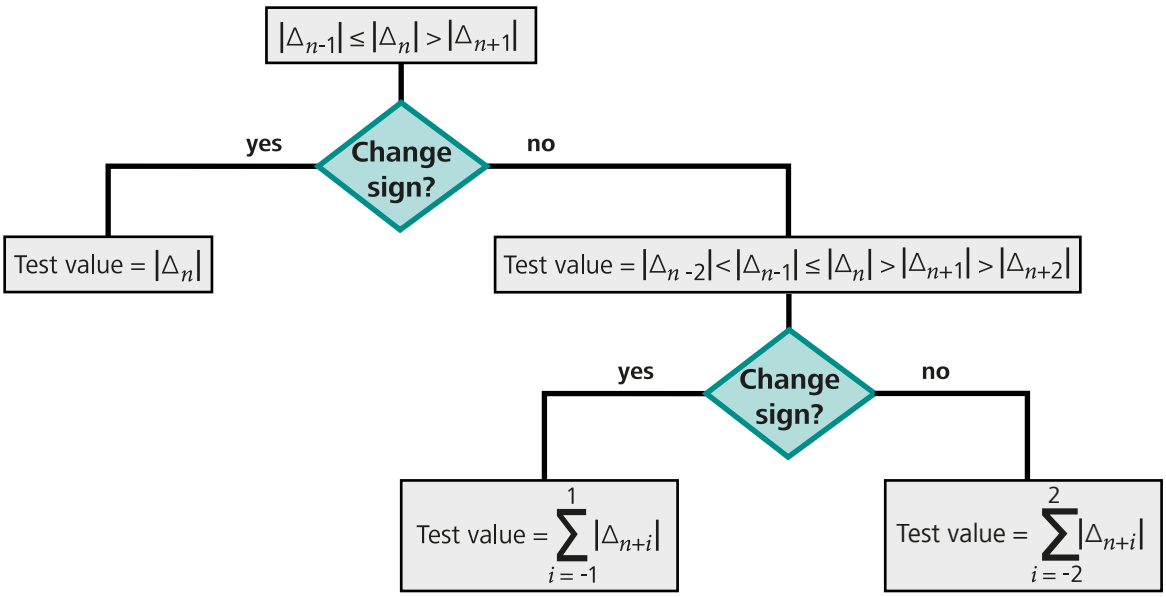
The EP criterion is a measure of the size of the jump in the titration curve. It is used to suppress the noise during the evaluation and to detect the relevant measurement jumps. In most applications, the default values are sufficient for this purpose.

The **ERC** (**E**quivalence point **R**ecognition **C**riterion) found for each jump is compared with the value specified in the **EP criterion** parameter. Equivalence points (EPs) where the ERC is smaller than the set EP criterion will not be recognized.

The appropriate value for the EP criterion can be calculated using the measuring point list:

1. Search for the largest measured value change Δ_n.

2. Use the measured value changes before and after Δ_n to calculate a series:
   $|\Delta_{n-2}|, |\Delta_{n-1}|, |\Delta_n|, |\Delta_{n+1}|, |\Delta_{n+2}|$
3. Based on the following chart, decide how many Δ values are needed to calculate the value for the EP criterion:



1. If a recognized EP is to be excluded, enter a value in the **EP criterion** parameter that is slightly higher than the calculated result.
2. If an unrecognized EP is to be taken into account, enter a value in the **EP criterion** parameter that is slightly lower than the calculated result.

Conductometric evaluation (only MET COND)

Conductometric evaluation allows the detection of multiple equivalence points without having to use window-based evaluation. It is carried out only at the end of titration and proceeds in 3 phases:

1. First, possible equivalence points are searched for based on the extreme points on the ERC (**E**quivalence point **R**ecognition **C**riterion) curve. The value in the **EP criterion** parameter is compared with the calculated ERC. Only extreme points where the absolute amount of ERC is greater than or equal to the defined EP criterion are considered.

2. A linear range is determined before and after the ERC extreme point. The linear range can be extended and shifted depending on the setting in the **Extension of the linear range** parameter.
   In the linear range, a linear regression according to the method of least squares is performed to determine the regression line. The position of the regression line is influenced by the **Weighting factor** parameter: If the parameter = 0, all measuring points in the linear range are weighted equally. The larger the weighing factor, the less measuring points in curved areas of the curve segment are taken into account.
3. The intersection point of the two regression lines before and after the corresponding ERC extreme point gives the position of the equivalence point on the volume axis.

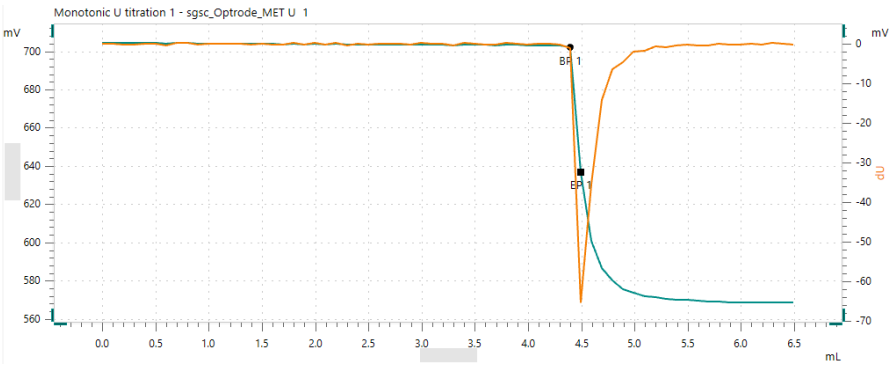
Artifacts at the beginning of the titration and noise can influence the evaluation of the titration curve. To minimize these unwanted effects, the following parameters can be used:

- **Evaluation start**: Volume at which the conductometric evaluation is started. The evaluation takes place after the measurement. Only measuring points whose volume is greater than or equal to the defined value are taken into account. Measurement points can thus be excluded from the evaluation.
- **Smoothing factor**: Factor that determines the smoothing of the titration curve. The higher this value, the more the noise is damped and the titration curve is smoothed. The smoothing of the titration curve has an influence on the ERC values and the drift and can cause a shift of the equivalence point.

To obtain reliable results, at least 15 measuring points before and after the ERC extreme point are required for the evaluation.

Break point evaluation

A break point evaluation is used to determine sharp changes of direction in the titration curve. This evaluation is suitable for photometric titrations.



See also

Curves – Gran evaluation (chapter 5.10.11.4, page 328)

MET – Command variables (chapter 5.11.8.4.3, page 492)

MET – Properties (chapter 5.11.8.4.1, page 472)

5.11.8.4.1 MET – Properties

The **MET** command is used for executing monotonic equivalence point titrations (**MET** = **M**onotonic **E**quivalence Point **T**itration).

Depending on the measured quantity required, the following commands can be selected:

- **MET COND**
  Monotonic equivalence point titration with conductivity measurement (measured quantity: Conductivity κ)
- **MET Ipol**
  Monotonic equivalence point titration with voltametric measurement with selectable polarization current (measured quantity: Potential U)
- **MET pH**
  Monotonic equivalence point titration with potentiometric pH measurement (measured quantity: pH)
- **MET U**
  Monotonic equivalence point titration with potentiometric potential measurement (measured quantity: Potential U)

The determination can be paused manually during the execution of a **MET** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

After selecting a **MET** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MET COND**, **MET Ipol**, **MET pH** and **MET U** commands:

Parameters

Start conditions	
Signal drift initial measured value	The initial measured value is applied as soon as the signal drift falls below the defined value or no later than after the maximum waiting time has expired. **Off** disables the drift control and the initial measured value is adopted after the maximum waiting time.

Start conditions	
Minimum waiting time	If drift control is enabled, the initial measured value will not be applied until after the minimum waiting time has expired at the earliest, and the measurement will be aborted, even if it has already fallen below the **Signal drift initial measured value**.
Maximum waiting time	**Drift control enabled:** If the signal drift does not fall below a defined value before the maximum waiting time has expired, then the initial measured value is adopted after the maximum waiting time has expired, and the measurement is aborted. **Drift control disabled:** The initial measured value is adopted after the maximum waiting time has expired and the measurement is canceled.
Start volume	The titrant is added before the start of titration until the start volume is reached. The following stop conditions are checked while dosing the start volume: ▪ **Stop volume** ▪ **Stop time**
Dosing rate start volume	Rate at which dosing takes place until the start volume has been reached. If, in the **Equipment** work area, a **Maximum dosing rate** is defined for dosing port 1 of the functional unit used that is smaller than the **Dosing rate start volume**, then the maximum dosing rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Start measured value (only for MET Ipol, MET pH and MET U)	The titrant is added before the start of titration until the start measured value is reached. The following stop conditions are checked while dosing the titrant: ▪ **Stop volume** ▪ **Stop measured value** ▪ **Stop time** **Off** disables this start condition. If the start measured value is already reached by dosing a start volume, then the start condition **Start measured value** is skipped. If the measured value does not change in this direction during dosing, then dosing is aborted without this start condition having been fulfilled.

Start conditions	
Dosing rate start measured value (only for MET Ipol, MET pH and MET U)	Rate at which dosing takes place until the start measured value has been reached. If, in the **Equipment** work area, a **Maximum dosing rate** is defined for dosing port 1 of the functional unit used that is smaller than the **Dosing rate start volume**, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Start slope (only for MET Ipol, MET pH and MET U)	The titrant is added until the start slope (measured value change per mL) is reached. The following stop conditions are checked while dosing the titrant: ▪ **Stop volume** ▪ **Stop measured value** ▪ **Stop time** **Off** disables this start condition.
Dosing rate start slope (only for MET Ipol, MET pH and MET U)	Rate at which dosing takes place until the start slope has been reached. If, in the **Equipment** work area, a **Maximum dosing rate** is defined for dosing port 1 of the functional unit used that is smaller than the **Dosing rate start volume**, then the maximum dosing rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Pause	Waiting time, e.g. for the measured value to stabilize after start or as reaction time after dosing a start volume. The pause follows at the end of all the start conditions.

Titration parameters	
Titration rate	The titration rate can either be determined using 3 predefined parameter sets, or the values for the titration parameters can be defined individually. ▪ **Slow**: Parameter set for titrations for which the finest details are to be visible. This can, however, lead to an increase in noise, which may result in unwanted equivalence points. ▪ **Optimal**: Parameter set that has been optimized for the most common applications. ▪ **Fast**: Parameter set for not very critical, fast titrations. ▪ **Enter values**: The values for the titration parameters must be defined individually. If a predefined parameter set is selected for the titration rate, the following parameters are displayed but they cannot be edited: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** ▪ **Volume increment** ▪ **Dosing rate** ▪ **Filling rate** The values used can be read in the corresponding parameters.
Signal drift	The measured value is adopted as soon as the signal drift falls below the defined value or no later than after the maximum waiting time has expired. Drift-controlled measured value acceptance is advisable if the time until a state of equilibrium is reached is variable. **Off** disables the drift control and the measured value is adopted after the maximum waiting time. This setting is useful if the reaction runs slowly or if the electrode is slow to respond.
Minimum waiting time	If drift control is enabled, then the measured value will not be applied until after the minimum waiting time has expired at the earliest, even if it has already fallen below the **Signal drift**.
Maximum waiting time	**Drift control enabled:** If the signal drift does not fall below a defined value before the maximum waiting time has expired, the measured value is adopted after the maximum waiting time has expired. **Drift control disabled:** The measured value is adopted after the maximum waiting time has expired.

Titration parameters	
Volume increment	Volume dosed at each dosing step. High accuracy requires using the correct volume increment. A good guide value for the volume increment is 0.1 mL. A total of 20 dosing steps is recommended until the equivalence point is reached. With greater consumption, the titration time can be optimized using the start conditions. Smaller volume increments (smaller than 0.1 mL) are required to determine blank values or to ensure accuracy with highly asymmetric curves. Larger volume increments are advisable for flatter curves. **Note**: The accuracy of the evaluation is not increased by using smaller increments, as the measured value change between 2 measuring points is then of the same order of magnitude as the noise. This means that unwanted equivalence points may be generated.
Dosing rate	Rate at which the volume increments are dosed. If a smaller **Maximum dosing rate** is defined for dosing port 1 of the used functional unit in the **Equipment** work area, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Filling rate	Rate at which the cylinder is filled. If, in the **Equipment** work area, a smaller **Maximum filling rate** is defined for the fill port for the functional unit used, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if air bubbles form during the aspiration of the solution, then the filling rate must be reduced accordingly so that the dosing drive is not overloaded.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.

Titration parameters	
Temperature	The input field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected.
I(pol) DC (only for MET Ipol)	The polarization current **I(pol) DC** (Direct Current) is the current that is applied to the polarizable electrode during voltametric measurement. **Note**: For OMNIS instruments, Metrohm recommends entering the current in increments of 0.5 µA. For instruments of the **Titrando** type an increment of 0.5 µA **must** be observed. For instruments of the **855 Robotic Titrosampler** type an increment of 2.5 µA **must** be observed.
Carry out electrode check (only for MET Ipol)	The electrode check is carried out for polarizable electrodes during the transition from an inactive normal status to the titration. It checks within a few seconds whether an electrode is connected and whether no short circuit is present.
Temperature compensation (only MET COND)	
Temperature compensation	Selection of the type of temperature compensation for the conductivity measurement during conductometric titration. ▪ **Constant factor**: If **Constant factor** is selected, then the following specific parameters appear: – **Reference temperature** – **Temperature coefficient** ▪ **DIN EN 27888**: This type of temperature compensation is used for the determination of ground water, spring water and surface water in accordance with DIN EN 27888. If **DIN EN 27888** is selected, the following specific parameter appears: – **Reference temperature** ▪ **No temperature compensation**
Reference temperature	The electrical conductivity depends greatly on the temperature. The conductivity measured at a particular temperature is automatically converted to the conductivity of this reference temperature (usually 20 °C or 25 °C).
Temperature coefficient	Temperature compensation is carried out with the constant factor entered here.
Stop conditions	
Stop volume	The titration is canceled as soon as the defined volume has been dosed since the start of the titration (including start conditions). The volume must be adjusted to the size of the titration vessel to prevent it from overflowing. In addition, the **Stop volume** should always be smaller than or equal to the cylinder volume to avoid refilling during the titration. **Off** disables this stop condition.

Stop conditions	
Stop measured value	The titration is canceled as soon as it falls below or exceeds the defined measured value since the start of the titration. Exceeding or falling below the stop measured value is monitored on the basis of the titration direction which is defined internally using the stop measured value and the start measured value (or the initial measured value if the start measured value is disabled). **Off** disables this stop condition.
Stop EP (only for MET Ipol, MET pH and MET U)	The titration is aborted as soon as the defined number of equivalence points (EP) has been evaluated according to the **EP criterion** parameter. **Off** disables this stop condition.
Volume after EP (only for MET Ipol, MET pH and MET U)	As soon as the number of equivalence points defined under **Stop EP** has been evaluated, the **Volume after EP** is added to the volume of the last equivalence point. The titration is canceled after this total volume has been dosed. Because determination of the equivalence point requires titration in excess of the equivalence point, the end volume will be greater than the equivalence point volume that leads to the action being canceled, even if **Volume after EP** = 0 mL. **Note**: This parameter was disabled in previous Metrohm applications with **"Off"**, which now corresponds to the setting "0 mL".
Stop time	The titration is canceled as soon as the defined time has elapsed since the start of the determination (including start conditions). **Off** disables this stop condition.

Potentiometric evaluation **(only MET Ipol, MET pH, MET U)**	
Selection of the type	Selection whether the equivalence points are evaluated and recognized throughout the entire titration curve (**Regular**) or only in certain segments of the curve (**Window-based**). The fields **EP criterion** and **EP recognition** only appear in the **Regular** setting. If **Window-based** is selected, then multiple evaluation windows can be defined or edited *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*.
EP criterion	Threshold value for the evaluation of equivalence points. Equivalence points are not evaluated if the calculated **ERC** value (ERC = **E**quivalence point **R**ecognition **C**riterion) is smaller than the defined value.

Potentiometric evaluation (only MET Ipol, MET pH, MET U)	
EP recognition	Filters for the recognition of equivalence points: ▪ **All** All evaluated equivalence points are recognized. ▪ **Last** Of the evaluated equivalence points, only the last is recognized. ▪ **Greatest** Of the evaluated equivalence points, only the one with the greatest ERC value (i.e. with the steepest curve section) is recognized. ▪ **Off** The evaluation and recognition of equivalence points is switched off.
[Edit evaluation windows]	The subsection for defining the evaluation windows is opened. *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*

Conductometric evaluation (only MET COND)	
Evaluation start	Volume at which the conductometric evaluation is started. The evaluation takes place after the titration. Only measuring points whose volume is greater than or equal to the defined value are taken into account.
Smoothing factor	Factor that determines the smoothing of the titration curve. The higher this value, the more the noise is damped and the titration curve is smoothed. The smoothing of the titration curve has an influence on the ERC curve and the drift and can cause a shift of the equivalence point. The value of the smoothing factor must not be higher than half of the number of measuring points. The maximum value is 25.
Extension of the linear range	Threshold value for the definition of the linear range before and after an ERC extreme point of the ERC curve. The linear range is extended to the point where the ERC value is smaller than the product of the entered percentage value and the ERC of the considered extreme point.
Weighting factor	Factor that determines to what extent measuring points in the curved areas of the titration curve are taken into account for the calculation of the regression line. The larger the factor, the less such measuring points are included. 0 means that all measuring points are weighted equally.

Conductometric evaluation (only MET COND)	
Selection of the type	Selection whether the equivalence points are evaluated and recognized throughout the entire titration curve (**Regular**) or only in certain segments of the curve (**Window-based**). The fields **EP criterion** and **EP recognition** only appear in the **Regular** setting. If **Window-based** is selected, then multiple evaluation windows can be defined or edited *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*.
EP criterion	Threshold value for the evaluation of equivalence points. Equivalence points are not evaluated if the calculated **ERC** value (ERC = **E**quivalence point **R**ecognition **C**riterion) is smaller than the defined value.
EP recognition	Filters for the recognition of equivalence points: ▪ **All** All evaluated equivalence points are recognized. ▪ **Last** Of the evaluated equivalence points, only the last is recognized. ▪ **Greatest** Of the evaluated equivalence points, only the one with the largest ERC value (i.e. with the sharpest break) is recognized.
[Edit evaluation windows]	The subsection for defining the evaluation windows is opened. *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*
Fixed point evaluation	
Define fixed points	The subsection for defining the fixed points is opened. *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*

Fixed point evaluation	
Specified quantity	Selection of the specified quantity for the evaluation of the fixed point from the measuring point list: Only valid for **MET COND**: ▪ **Conductivity κ** The values **Temperature**, **Volume** and **Time** are interpolated from the measuring point list for the specified conductivity κ. ▪ **Time** The values **Conductivity κ**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Conductivity κ**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume. Only valid for **MET Ipol**: ▪ **Potential** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume. Only valid for **MET pH**: ▪ **pH** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified pH value. ▪ **Time** The values **pH**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **pH**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume. Only valid for **MET U**: ▪ **Potential** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume.
Fixed point at	Specified measured value for the evaluation of the fixed point.

Break point evaluation	
Selection of the type	Selection whether the break points are evaluated throughout the entire titration curve (**Regular**) or only in certain segments of the curve (**Window-based**) or not at all (**Off**). If **Window-based** is selected, then multiple evaluation windows can be defined or edited: *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*.
BP criterion	Criterion for the evaluation of break points. Standardized difference between maximum and minimum of the second derivative. Break points with a found **BRC** value (BRC = **B**reakpoint **R**ecognition **C**riterion) that is smaller than the value entered here will not be evaluated.
Min. deflection	Threshold value of the slope difference between the sections before and after the break point. The smaller the difference, the more break points will be evaluated.
Max. expected BPs	Maximum number of break points that are expected. The curve is smoothed until the number of evaluated break points is smaller or equal to this number.
BP recognition	Filters for the recognition of break points: ▪ **First** Of the evaluated break points, only the first one is recognized. ▪ **Last** Of the evaluated break points, only the last one is recognized.
[Edit evaluation windows]	The subsection for defining the evaluation windows is opened. *(see "Curves – Window-based evaluation", chapter 5.10.11.2, page 325)*

Gran evaluation **(only MET pH)**	
Selection of the type	Selection as to whether the titration curve is evaluated according to the Gran procedure (**Gran point**) or not (**Off**). If **Gran point** is selected, then a Gran point is determined for the titration.
Reaction type	Selection of the reaction type (analyte, titrant). The available options for the parameter **Gran plot** are displayed, depending on the selection. ▪ **Weak monoprotic acid, strong base**: Titration of a weak monoprotic acid with a strong base. ▪ **Weak monoprotic base, strong acid**: Titration of a weak monoprotic base with a strong acid. ▪ **Strong base, strong acid or strong acid, strong base**: Titration of a strong base with a strong acid or a strong acid with a strong base.

Gran evaluation (only MET pH)	
Gran plot	Range of the titration curve that is used to determine the Gran point. Specifying the lower limit and the upper limit for the selected segment makes it possible to define the linear range in which the measuring points for the determination of the regression line are used. Depending on the selection of the reaction type, the parameters for the Gran function used for the evaluation can also be defined. ▪ **Acidic segment**: If the analyte is acidic, then the segment is used before the equivalence point. If the analyte is alkaline, then the segment after the equivalence point is used. If **Acidic segment** is selected, the following specific parameters appear: – **Initial volume** (does not apply for Weak monoprotic acid, strong base) – **Lower limit pH acidic** – **Upper limit pH acidic** ▪ **Alkaline segment**: If the analyte is acidic, then the segment after the equivalence point is used. If the analyte is alkaline, then the segment before the equivalence point is used. If **Alkaline segment** is selected, the following specific parameters appear: – **Initial volume** (does not apply for Weak monoprotic base, strong acid) – **Lower limit pH alkaline** – **Upper limit pH alkaline** ▪ **Acidic and alkaline segment**: Not only the segment before the equivalence point but also the segment after the equivalence point are both used. If **Acidic and alkaline segment** is selected, the following specific parameters appear: – **Initial volume** – **Lower limit pH acidic** – **Upper limit pH acidic** – **Lower limit pH alkaline** – **Upper limit pH alkaline** **Note**: The **Lower limit pH** and the **Upper limit pH** must be defined for each segment in such a way that both limits are located on the same side of the equivalence point. ▪ **Normalized**: The entire titration curve is used. The standardized procedure is available only for the reaction type **Strong base, strong acid or strong acid, strong base**. If **Normalized** is selected, the following specific parameters appear: – **Initial volume** – **Lower limit pH** – **Upper limit pH** **Note**: The selection **Normalized** corresponds to the evaluation procedure in previous Metrohm applications. Additional information regarding the Gran functions applied: *(see "Curves – Gran evaluation", chapter 5.10.11.4, page 328)*

Gran evaluation (only MET pH)	
Initial volume	Volume of the analyte that is in the sample vessel before the titration is started.
Lower limit pH acidic, **Lower limit pH alkaline** or **Lower limit pH**	Defines the lower limit of the range in which the measuring points for determining the regression line are used.
Upper limit pH acidic, **Upper limit pH alkaline** or **Upper limit pH**	Defines the upper limit of the range in which the measuring points for determining the regression line are used.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: Only valid for **MET COND**: ▪ **Conductivity κ** ▪ **ERC** Only valid for **MET Ipol**: ▪ **Potential** ▪ **dU** Only valid for **MET pH**: ▪ **pH** ▪ **dpH** ▪ **Gran function value** Only valid for **MET U**: ▪ **Potential** ▪ **dU** Valid for all commands: ▪ **Volume** (default value) ▪ **Time** ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: Only valid for **MET COND**: ▪ **Conductivity κ** (default value) If **Conductivity κ** is selected, the following specific parameter appears: – **Displaying regression lines** ▪ **ERC** Only valid for **MET Ipol**: ▪ **Potential** (default value) ▪ **dU** Only valid for **MET pH**: ▪ **pH** (default value) ▪ **dpH** ▪ **Gran function value** If **Gran function value** is selected, the following specific parameter appears: – **Displaying regression lines** Only valid for **MET U**: ▪ **Potential** (default value) ▪ **dU** Valid for all commands: ▪ **Volume** ▪ **Time** ▪ **Temperature**
Displaying regression lines (only for MET COND and MET pH)	Display of at least one regression line that runs through the values of the selected quantity. The check box is used for activation. The regression lines are displayed only if the quantity **Conductivity κ** (MET COND) or **Gran function value** (MET pH)is selected for the corresponding y-axis or y2-axis and the quantity **Volume** is selected for the x-axis. The display is disabled by default. In addition, the measuring points (MET COND) or Gran function values (MET pH) used for the calculation of the regression line are highlighted. For a Gran evaluation, the volume of the Gran point is also shown as a vertical line. **NOTICE**: Depending on the command, 1 or 2 regression lines are displayed.

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.

Chart – y2-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: Only valid for **MET COND**: ▪ **Conductivity κ** ▪ **ERC** (default value) Only valid for **MET Ipol**: ▪ **Potential** ▪ **dU** (default value) Only valid for **MET pH**: ▪ **pH** ▪ **dpH** (default value) ▪ **Gran function value** If **Gran function value** is selected, the following specific parameter appears: – **Displaying regression lines** Only valid for **MET U**: ▪ **Potential** ▪ **dU** (default value) Valid for all commands: ▪ **Volume** ▪ **Time** ▪ **Temperature**
Displaying regression lines (only for MET COND and MET pH)	Display of at least one regression line that runs through the values of the selected quantity. The check box is used for activation. The regression lines are displayed only if the quantity **Conductivity κ** (MET COND) or **Gran function value** (MET pH)is selected for the corresponding y-axis or y2-axis and the quantity **Volume** is selected for the x-axis. The display is disabled by default. In addition, the measuring points (MET COND) or Gran function values (MET pH) used for the calculation of the regression line are highlighted. For a Gran evaluation, the volume of the Gran point is also shown as a vertical line. **NOTICE**: Depending on the command, 1 or 2 regression lines are displayed.

Curve simulation	
Curve selection	Simulated curves can be used with OMNIS instruments to check the determination run. The titration sequence is defined by the set parameters. The simulation must be deactivated before analyzing real samples. Selection of the simulation curve: ▪ **None** (default value) The curve simulation is disabled. ▪ **Hydrochloric acid** Simulation curve of the titration of hydrochloric acid with caustic soda (titration curve with one equivalence point). ▪ **Citric acid** (only MET Ipol, MET pH and MET U) Simulation curve of the titration of citric acid with caustic soda (titration curve with 3 equivalence points). ▪ **Alpha acid in hops** (only MET COND) Simulation curve of the titration of alpha acid in hops with lead acetate solution (titration curve with one equivalence point).

The curve simulation cannot be used for instruments of the **Titrando** and **855 Robotic Titrosampler** type.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift initial measured value**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Dosing rate start volume**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Start measured value**
  Minimum value: –1,200.0 mV
  Maximum value: 1,200.0 mV
- **Start measured value pH**
  Minimum value: –13.000
  Maximum value: 20.000
- **Dosing rate start measured value**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)

- **Dosing rate start slope**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Signal drift**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Dosing rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **I(pol) DC** (Titrando)
  Minimum value: –122.5 µA
  Maximum value: 122.5 µA
  Permitted increment: 0.5 µA
- **I(pol) DC** (855 Robotic Titrosampler)
  Minimum value: –122.5 µA
  Maximum value: 122.5 µA
  Permitted increment: 2.5 µA
- **Filling rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Stop measured value**
  Minimum value: –1,200.0 mV
  Maximum value: 1,200.0 mV
- **Stop measured value pH**
  Minimum value: –13.000
  Maximum value: 20.000
- **Fixed point at**
  Minimum value MET Ipol and MET U: –1,200.0 mV
  Maximum value MET Ipol and MET U: 1,200.0 mV
  Minimum value MET pH: –13.000
  Maximum value MET pH: 20.000

Execute with

In order for a **MET** command to be executed, the corresponding functional units and, for analog measuring inputs, the required sensor need to be assigned to the command.

- Dosing unit or buret to which the titrant is connected:
  Dosing Drive with connected **Cylinder Unit**, **800 Dosino** with connected **807 Dosing Unit**, **805 Dosimat** with connected **806 Exchange Unit** or **Internal Dosing Drive** with connected **806 Exchange Unit**

- Measuring input (digital or analog) to which the sensor required for the titration is connected:
  Measuring Module Digital, **Measuring Module Conductivity**, **Measuring Module Analog**, **Measuring Interface iConnect**, **Measuring Interface Analog** or **Measuring Interface Conductivity**
- Sensor (digital, intelligent or analog):
  Polarizable metal electrode, **Ion-selective electrode**, **pH electrode**, **Metal electrode** or **Other sensor**

After a functional unit for the command has been selected, the following additional parameters appear:

For **Dosing Drive**:	
Dosing port	Port that is to be used to dose the defined volume increment. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1 (default value). ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2.

For **Measuring Module Analog**:	
Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input (only for MET pH and MET U)	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **Difference**: Differential measurement between electrodes at INPUT 1 and INPUT 2.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error. **Note**: For a combined pH/temperature sensor, both measuring inputs must be set to **INPUT 1**.

Measuring input (only for MET pH and MET U)	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.

For **Measuring Module Conductivity** (MET COND):	
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

For **Measuring Interface Analog** and **Measuring Interface iConnect** (MET pH and MET U):	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **Ind./Ref./Temp.**: Measurement with an analog electrode. ▪ **iConnect**: Measurement with an intelligent electrode (iTrode)
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Measuring Interface Analog** (MET Ipol):	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: **Pol./Temp.**: Measurement with a polarizable electrode.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Measuring Interface Conductivity** (MET COND):	
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Curves – Fixed point evaluation (chapter 5.10.11.3, page 327)

Curves – Window-based evaluation (chapter 5.10.11.2, page 325)

DET – Properties (chapter 5.11.8.3.1, page 445)

KFC – Properties (chapter 5.11.8.11, page 586)

KFT – Properties (chapter 5.11.8.10.1, page 568)

MET – Command variables (chapter 5.11.8.4.3, page 492)

MET – Principle (chapter 5.11.8.4, page 468)

MET – Run (chapter 5.11.8.4.2, page 491)

SET – Properties (chapter 5.11.8.6.1, page 512)

Sensor – Definition (chapter 5.12.6, page 998)

5.11.8.4.2 MET – Run

The **MET** command is executed in 4 steps:

1 – Determining the initial measured value

The initial measured value (measured value before start of pre-dosing) is determined according to the parameters in the parameter group **Start conditions**, either drift-controlled or after a maximum waiting time has elapsed.

2 – Processing the start conditions

If a **Start volume** was defined in **Start conditions**, it will be dosed before the actual titration.

For the **MET Ipol**, **MET pH** and **MET U** commands, the start conditions are checked afterwards in the following order: **Start volume** ➔ **Start measured value (pH)** ➔ **Start slope (pH)**

The defined **Pause** time is then observed.

3 – Carrying out the titration

The titration is carried out and evaluated according to the parameters defined under **Titration parameters** and **Potentiometric evaluation** (MET Ipol, MET pH, MET U) or **Conductometric evaluation** (MET COND).

- **Fixed point evaluation**
  Optionally, up to 9 fixed points can be defined in **Fixed point evaluation** that are calculated from the measuring point list during the titration.
- **Break point evaluation**
  The titration curve can be optionally evaluated according to the parameters defined under **Break point evaluation**.
- **Gran evaluation** (only MET pH)
  The titration curve can be optionally evaluated according to the parameters defined under **Gran evaluation**.
- **Chart – … axes**
  Different quantities can be selected for the x-axis and y-axis. A y2-axis can be displayed as an option.

4 – Completing the titration

The titration is completed as usual as soon as the first stop condition defined in **Stop conditions** is reached.

A running titration can be canceled by a manual cancellation or with the emergency stop or in case of an error.

See also

MET – Command variables (chapter 5.11.8.4.3, page 492)

MET – Principle (chapter 5.11.8.4, page 468)

MET – Properties (chapter 5.11.8.4.1, page 472)

5.11.8.4.3 MET – Command variables

The following variables are generated by the commands **MET COND**, **MET Ipol**, **MET pH** and **MET U** in the process sequence and can be used in a formula under the designation '**Variable name**.*Command name*'.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**ERC.EP{x}**.*Command name*' (x = 1–9) Calculated ERC value for the equivalence point. If this value is greater than or equal to the value defined in the **EP criterion** parameter, then the equivalence point will be recognized.
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**GranFunctionvalue.GP{x}**.*Command name*' (x = 1–9) Function value of the Gran point.
'**Index.BP{x}**.*Command name*' (x = 1–9) Index of the break point.
'**Index.EP{x}**.*Command name*' (x = 1–9) Index of the equivalence point.
'**Index.FP{x}**.*Command name*' (x = 1–9) Index of the fixed point.
'**Index.GP{x}**.*Command name*' (x = 1–9) Index of the Gran point.
'**InterceptAcidicSegment.GP{x}**.*Command name*' (x = 1–9) y-intercept of the regression line in the acidic segment of the Gran plot.
'**InterceptAlkalineSegment.GP{x}**.*Command name*' (x = 1–9) y-intercept of the regression line in the alkaline segment of the Gran plot.
'**Measvalue.BP{x}**.*Command name*' (x = 1–9) Measured value of the break point. Unit: Defined in the '**Unit.Measvalue**' variable

Command variables
'**Measvalue.EP{x}**.*Command name*' (x = 1–9) Measured value of the equivalence point. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.FP{x}**.*Command name*' (x = 1–9) Measured value of the fixed point. Unit: None (MET pH) or mV (MET U, MET Ipol)
'**Measvalue.GP{x}**.*Command name*' (x = 1–9) Measured value of the Gran point.
'**NumberOfDataPointsAcidicSegment.GP{x}**.*Command name*' (x = 1–9) Number of Gran function values that are used to calculate the regression line in the acidic segment of the Gran plot.
'**NumberOfDataPointsAlkalineSegment.GP{x}**.*Command name*' (x = 1 … 9) Number of Gran function values that are used to calculate the regression line in the alkaline segment of the Gran plot.
'**SlopeAcidicSegment.GP{x}**.*Command name*' (x = 1–9) Slope of the regression line in the acidic segment of the Gran plot.
'**SlopeAlkalineSegment.GP{x}**.*Command name*' (x = 1–9) Slope of the regression line in the alkaline segment of the Gran plot.
'**SumOfSquaredErrorsAcidicSegment.GP{x}**.*Command name*' (x = 1 … 9) Sum of squares of the residuals, i.e. the deviation between the Gran function value and the corresponding point on the regression line, in the acidic segment of the Gran plot. The smaller the value, the better the regression line calculated by the regression analysis matches the corresponding segment of the Gran plot. The standard deviation can be calculated from the error sum of squares and the number of Gran function values considered for the regression line.
'**SumOfSquaredErrorsAlkalineSegment.GP{x}**.*Command name*' (x = 1 … 9) Sum of squares of the residuals, i.e. the deviation between the Gran function value and the corresponding point on the regression line, in the alkaline segment of the Gran plot. The smaller the value, the better the regression line calculated by the regression analysis matches the corresponding segment of the Gran plot. The standard deviation can be calculated from the error sum of squares and the number of Gran function values considered for the regression line.
'**Temperature.BP{x}**.*Command name*' (x = 1–9) Temperature associated with the break point. Unit: °C

Command variables
'**Temperature.EP{x}**.*Command name*' (x = 1–9) Temperature associated with the equivalence point. Unit: °C
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Temperature.FP{x}**.*Command name*' (x = 1–9) Temperature associated with the fixed point. Unit: °C
'**Temperature.GP{x}**.*Command name*' (x = 1–9) Temperature associated with the Gran point. Unit: °C
'**Time.BP{x}**.*Command name*' (x = 1–9) Time stamp associated with the break point. Unit: s
'**Time.EP{x}**.*Command name*' (x = 1–9) Time stamp associated with the equivalence point. Unit: s
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Time.FP{x}**.*Command name*' (x = 1–9) Time stamp associated with the fixed point. Unit: s
'**Time.GP{x}**.*Command name*' (x = 1–9) Time stamp associated with the Gran point. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of the measured values: None (MET pH) or mV (MET U, MET Ipol) or mS/cm (MET COND)
'**Volume.BP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the break point is reached. Unit: mL

Command variables
'**Volume.EP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the equivalence point is reached. Unit: mL
'**Volume.Final**.*Command name*' End volume after processing the command, i.e. total dosed volume at the end of the command. Unit: mL
'**Volume.FP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the fixed point is reached. Unit: mL
'**Volume.GP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the Gran point is reached. Unit: mL

In the case of variables with index **{x}**, the index **{1}** is set automatically at the time of insertion in a formula. This index can be set manually to 2–9 (e.g. '**Volume.EP{3}**.*Command name*' for the volume of the third equivalence point).

Equipment variables
'**Concentration.CurrentSolution**.*Command name*' Concentration of the solution used that is dosed with the dosing unit or buret (corresponds to the concentration of component 1 in the solution used). Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable
'**Diameter.AspirationTube.CurrentSolution**.*Command name*' Diameter of the aspiration tubing that is connected to the Liquid Adapter. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the Liquid Adapter. Unit: cm
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.
'**Name.CurrentSolution**.*Command name*' Name of the solution used with the dosing unit.

Equipment variables
'**Slope.CurrentSensor**.*Command name*' Quotient from the slope of the sensor used and the Nernst slope with the respective temperature. This variable is available only for pH electrodes. Unit: Determined by the sensor used.
'**Titer.CurrentSolution**.*Command name*' Titer of the solution connected to the Liquid Adapter that is dosed with the dosing unit. The titer is the factor that indicates the deviation of the actual concentration from the nominal concentration of a solution. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Concentration unit of the solution that is dosed with the dosing unit (corresponds to the concentration unit of component 1 in the solution). The unit is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer of the solution that is connected to the Liquid Adapter and that is dosed with the dosing unit.
'**ZeroPoint.CurrentSensor**.*Command name*' Electrode zero point of the sensor used. This variable is available only for pH electrodes. Unit: Determined by the sensor used.

See also

MET – Principle (chapter 5.11.8.4, page 468)

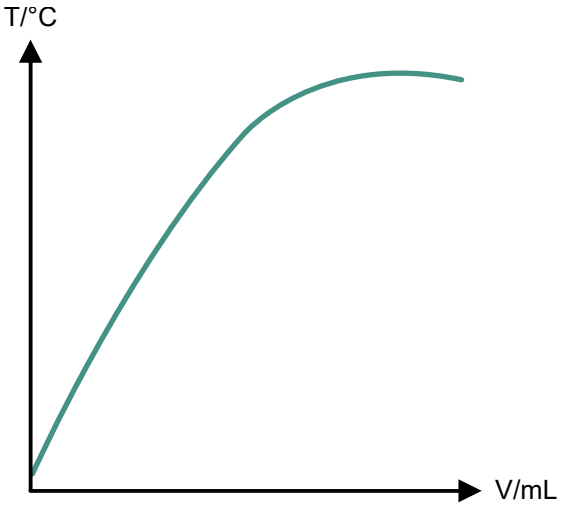
MET – Properties (chapter 5.11.8.4.1, page 472)

MET – Run (chapter 5.11.8.4.2, page 491)

5.11.8.5 TET – Principle

Measuring principle

Titrations with constant reagent addition and continuous temperature measurement are carried out with the **TET** command. The titration is canceled as soon as the first stop condition is reached.



Thermometric evaluation

The titration curve and the ERC curve (ERC = **E**quivalence point **R**ecognition **C**riterion) are automatically evaluated during and after the titration. All extreme points on the ERC curve are possible equivalence points that can be recognized by EP conditions. The EP conditions are defined in the parameters of the **TET** command and consist of a reaction type and an EP criterion. The EP criterion serves as a threshold value for the ERC value of the possible equivalence point.

After titration, an internal system list of possible equivalence points is generated, which is sorted before equivalence point recognition according to the type defined by the user: By ascending volume or by descending peak height. In the next step, the defined EP conditions are compared in sequence from top to bottom with the sorted list of possible equivalence points. As soon as the first EP condition is fulfilled by a possible equivalence point, i.e. the absolute value of the ERC value of the possible equivalence point is greater than the absolute value of the EP criterion, the equivalence point is recognized and receives the same index as the fulfilled EP condition. In the further procedure, the next EP condition is then compared with the list of possible equivalence points from which the recognized equivalence points have been removed. If an EP condition is not fulfilled by any possible equivalence point, its index is not assigned.

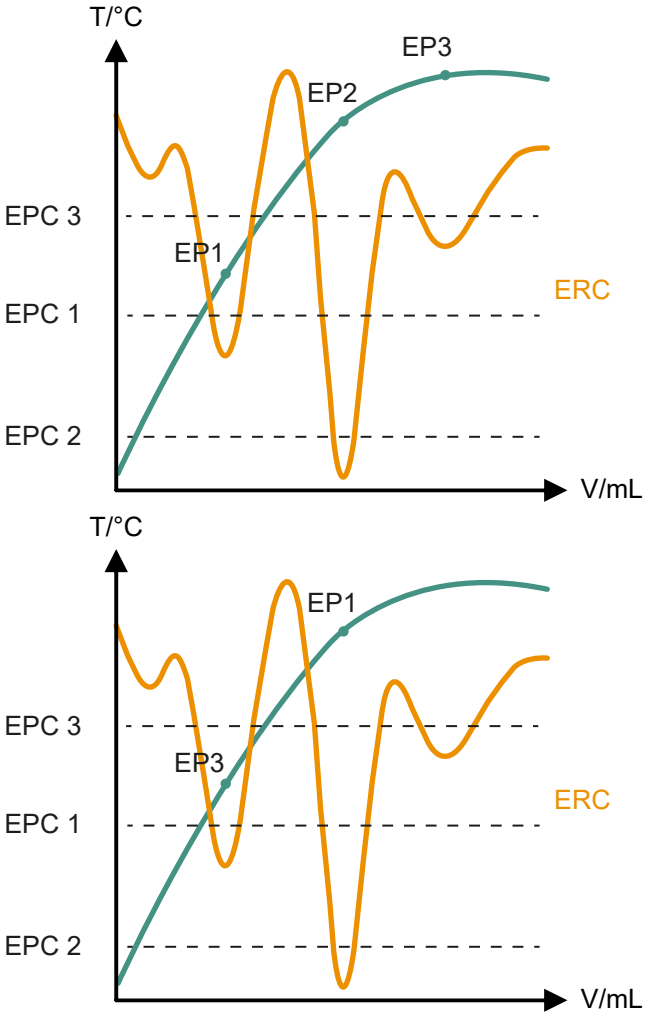
Titration artifacts at the beginning of the measurement and noise can influence the automatic evaluation of the titration curve. To minimize this influence, the following parameters can be set:

- **Filtering factor**
- **Damping until**

Examples

The following examples show the effect of sorting the possible equivalence points on their recognition. In the first example, the EP criteria (EPC

1–3) of the defined EP conditions are compared with the list of possible equivalence points sorted by ascending volume. One equivalence point is recognized for each EP condition. In the second example, the same EP conditions are compared with the list of possible equivalence points sorted by descending peak height. The first EP condition is fulfilled by the possible equivalence point with the largest peak height, while the second EP condition cannot be fulfilled by any other possible equivalence point.

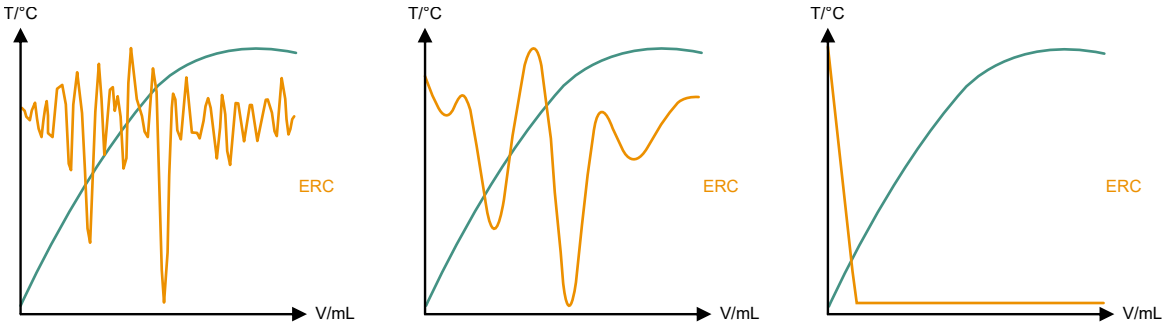


Filtering factor

The titration curve can be smoothed by the filtering factor. The higher the value for the filtering factor, the more the noise is damped and the titration curve is smoothed. The smoothing of the titration curve has an influence on the ERC curve and the slope and can cause a shift of the equivalence point.

Examples

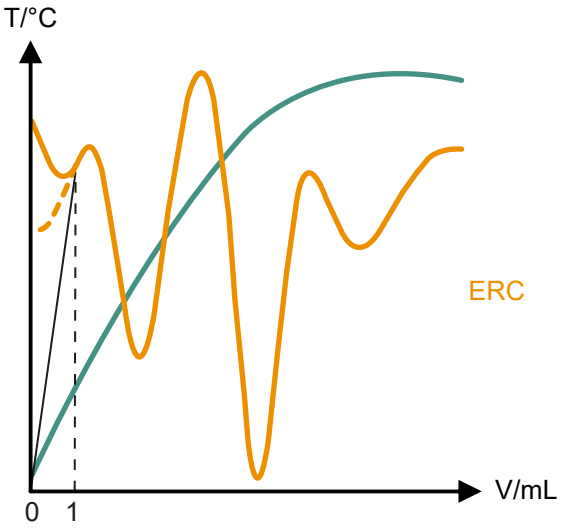
Filtering factor 20, filtering factor 50 and filtering factor 100.



Further information on the optimal setting of the filtering factor: *Practical thermometric titrimetry*.

Damping until

The ERC curve can be damped from the start of the measurement to the dosing of a defined volume. The damping minimizes the influence of titration artifacts (e.g. outliers) that occur at the beginning of the measurement and could be misinterpreted as equivalence points. It is a linear function with a positive slope, i.e. its influence is greatest at the start of the measurement and decreases linearly up to the defined volume. For this purpose, the first measuring point is multiplied by 0 and the last measuring point before the defined volume is multiplied by 1. The measuring points in between are each multiplied in linear ascending order by the corresponding value between 0 and 1.



Titer determination

For titer determination with the **TET** command, a linear regression can be performed via multiple subsamples with different sample sizes of the primary standard with the **EVAL LINEAR REGRESSION** command. If the sample size is recorded for the x-axis with a **CALC** command and the volume of the end point of the titration is recorded for the y-axis with another **CALC** command, the command variable '**Slope.Result**.*Com-*

mand name' outputs the slope which can be used for the calculation of the titer.

Blank value determination

For the blank value determination with the **TET** command, a linear regression can be performed via multiple subsamples with different sample quantities with the **EVAL LINEAR REGRESSION** command. If the sample size is recorded for the x-axis with a **CALC** command and the volume of the end point of the titration is recorded for the y-axis with another **CALC** command, the command variable '**Intercept.Result**.*Command name*' outputs the y-intercept which corresponds to the blank value. The blank value can be positive or negative.

See also

EVAL LINEAR REGRESSION – Parameters (chapter 5.11.8.68, page 776)

TET – Command variables (chapter 5.11.8.5.3, page 507)

TET – Properties (chapter 5.11.8.5.1, page 501)

5.11.8.5.1 TET – Properties

The **TET** command is used for executing thermometric equivalence point titrations (**TET** = **T**hermometric **E**quivalence Point **T**itration).

After selecting the **TET** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **TET** command:

Parameters

Start conditions	
Start volume	The titrant is added before the start of titration until the start volume is reached. The following stop conditions are checked while dosing the start volume: ▪ **Stop volume** ▪ **Stop time** The volume dosed during titration must always be smaller than or equal to the cylinder volume. Refilling during titration is not possible.

Start conditions	
Dosing rate start volume	Rate at which dosing takes place until the start volume has been reached. If, in the **Equipment** work area, a **Maximum dosing rate** is entered for dosing port 1 of the functional unit used that is smaller than the **Dosing rate start volume**, then the maximum dosing rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Pause	Waiting time, e.g. for the measured value to stabilize after start or as reaction time after dosing a start volume. The pause follows at the end of all the start conditions.

Titration parameters	
Dosing rate	Rate at which the volume increments are dosed. If a smaller **Maximum dosing rate** is defined for dosing port 1 of the used functional unit in the **Equipment** work area, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Filling rate	Rate at which the cylinder is filled. If, in the **Equipment** work area, a smaller **Maximum filling rate** is defined for the fill port for the functional unit used, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if air bubbles form during the aspiration of the solution, then the filling rate must be reduced accordingly so that the dosing drive is not overloaded.

Stop conditions	
Stop volume	The titration is canceled as soon as the defined volume has been dosed since the start of the titration (including start conditions). The volume must be adjusted to the size of the titration vessel to prevent it from overflowing. In addition, the **Stop volume** must always be smaller than or equal to the cylinder volume. Refilling during titration is not possible. **Off** disables this stop condition.
Stop measured value	The titration is canceled as soon as it falls below or exceeds the defined measured value since the start of the titration. Exceeding or falling below the stop measured value is monitored on the basis of the titration direction which is defined internally using the stop measured value and the initial measured value. **Off** disables this stop condition.
Stop time	The titration is canceled as soon as the defined time has elapsed since the start of the determination (including start conditions). **Off** disables this stop condition.
Stop slope mode	Mode that determines the stop condition for the slope (for temperature versus volume). ▪ **Off**: The stop condition is disabled. ▪ **Less than**: The titration is canceled as soon as the slope falls below the defined stop slope. ▪ **Greater than**: The titration is canceled as soon as the slope exceeds the defined stop slope. If **Less than** or **Greater than** is selected, the following specific parameters appear: – **Stop slope** – **Stop slope active after**
Stop slope	The titration is canceled as soon as the slope falls below or exceeds the defined stop slope depending on the selection in parameter **Stop slope mode**.
Stop slope active after	The titration will be canceled after reaching the stop condition for the slope only if the defined volume has already been added.
Additional volume after stop	As soon as the stop condition **Stop measured value**, **Stop time** or **Stop slope** is reached, the defined additional volume is dosed and the titration is then canceled.

Thermometric evaluation	
Filtering factor	Factor that determines the smoothing of the titration curve. The higher this value, the more the noise is damped and the titration curve is smoothed. The smoothing of the titration curve by the filtering factor has an influence on the ERC curve and the slope and can cause a shift of the equivalence point. Additional information on the filtering factor: *(see "TET – Principle", chapter 5.11.8.5, page 497)*
Damping until	The ERC curve is dampened from the start of the measurement to the defined volume. The start volume is not taken into account at this time. The damping minimizes the influence of titration artifacts (e.g. outliers) that occur at the beginning of the measurement and could be misinterpreted as equivalence points. It is a linear function with a positive slope, i.e. its influence is greatest at the start of the measurement and decreases linearly up to the defined volume. The defined volume must be before the first equivalence point. Additional information on damping: *(see "TET – Principle", chapter 5.11.8.5, page 497)*
Evaluation start	The thermometric evaluation starts as soon as the defined volume has been dosed since the start of the titration (including start conditions).
Sort equivalence points by	For the recognition of the equivalence points, they are compared with the defined EP conditions according to the selected sorting. ▪ **Volume (ascending)**: The possible equivalence points are sorted by increasing volume. ▪ **Peak height (descending)**: The possible equivalence points are sorted by decreasing peak height. Additional information on the thermometric evaluation: *(see "TET – Principle", chapter 5.11.8.5, page 497)*
Define EP conditions	The window for defining the conditions for equivalence points is opened: *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*
Fixed point evaluation	
Define fixed points	The window for defining the fixed points is opened. *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*

Fixed point evaluation	
Specified quantity	Selection of the specified quantity for the evaluation of the fixed point from the measuring point list: ▪ **Temperature** The values **Time** and **Volume** are interpolated from the measuring point list for the specified temperature. ▪ **Time** The values **Temperature** and **Volume** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Temperature** and **Time** are interpolated from the measuring point list for the specified volume.
Fixed point at	Specified measured value for the evaluation of the fixed point.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Volume** (default value) ▪ **Temperature** ▪ **Slope** ▪ **ERC** ▪ **Time**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Volume** ▪ **Temperature** (default value) ▪ **Slope** ▪ **ERC** ▪ **Time**

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Volume** ▪ **Temperature** ▪ **Slope** ▪ **ERC** (default value) ▪ **Time**

Curve simulation	
Curve selection	Simulated curves can be used with OMNIS instruments to check the determination run. The titration sequence is defined by the set parameters. The simulation must be deactivated before analyzing real samples. Selection of the simulation curve: ▪ **None** (default value) The curve simulation is disabled. ▪ **Hydrochloric acid** Simulation curve of the titration of hydrochloric acid with caustic soda (titration curve with one equivalence point). ▪ **Phosphoric acid** Simulation curve of the titration of phosphoric acid with caustic soda (titration curve with 3 equivalence points). ▪ **Calcium and magnesium in milk** Simulation curve of the titration of milk and trichloroacetic acid with tetrasodium EDTA (titration curve with 2 equivalence points).

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **TET** command to be executed, the corresponding functional units need to be assigned to the command.

- Dosing unit to which the titrant is connected:
  Dosing Drive with connected **Cylinder Unit**
- Measuring input to which the digital sensor of the **Thermoprobe** type required for the titration is connected:
  Measuring Module Digital

After a functional unit for the command has been selected, the following additional parameters appear:

For **Dosing Drive**:	
Dosing port	Port that is to be used to dose a volume. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1 (default value). ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Curves – Fixed point evaluation (chapter 5.10.11.3, page 327)

Curves – Thermometric evaluation (chapter 5.10.11.5, page 331)

Sensor – Definition (chapter 5.12.6, page 998)

TET – Command variables (chapter 5.11.8.5.3, page 507)

TET – Principle (chapter 5.11.8.5, page 497)

TET – Run (chapter 5.11.8.5.2, page 507)

5.11.8.5.2 TET – Run

The **TET** command is executed in 3 steps:

1 – Processing the start conditions

If a **Start volume** was defined in **Start conditions**, it will be dosed before the actual titration.

The defined **Pause** time is then observed.

2 – Carrying out the titration

The titration is carried out and evaluated according to the parameters defined under **Titration parameters** and **Thermometric evaluation**.

- **Fixed point evaluation**
  Optionally, up to 9 fixed points can be defined in **Fixed point evaluation** that are calculated from the measuring point list during the titration.
- **Chart – … axes**
  Different quantities can be selected for the x-axis and y-axis. A y2-axis can be displayed as an option.

3 – Completing the titration

The titration is completed as usual as soon as the first stop condition defined in **Stop conditions** is reached.

A running titration can be canceled by a manual cancellation or with the emergency stop or in case of an error.

See also

TET – Command variables (chapter 5.11.8.5.3, page 507)

TET – Principle (chapter 5.11.8.5, page 497)

TET – Properties (chapter 5.11.8.5.1, page 501)

5.11.8.5.3 TET – Command variables

The following variables are generated by the **TET** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**ERC.EP{x}**.*Command name*' (x = 1–9) Calculated ERC value for the equivalence point. If this value is greater than or equal to the threshold value defined in the **EP criterion** parameter, then the equivalence point will be recognized.
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Index.EP{x}**.*Command name*' (x = 1–9) Index of the equivalence point.
'**Index.FP{x}**.*Command name*' (x = 1–9) Index of the fixed point.
'**Measvalue.EP{x}**.*Command name*' (x = 1–9) Measured value of the equivalence point. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.FP{x}**.*Command name*' (x = 1–9) Measured value of the fixed point. Unit: Defined in the '**Unit.Measvalue**' variable
'**Slope.Final**.*Command name*' End value of the slope after processing the command. Unit: °C/mL
'**Time.EP{x}**.*Command name*' (x = 1–9) Time stamp associated with the equivalence point. Unit: s

Command variables
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Time.FP{x}**.*Command name*' (x = 1–9) Time stamp associated with the fixed point. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of the measured value.
'**Volume.EP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the equivalence point is reached. Unit: mL
'**Volume.Final**.*Command name*' End volume after processing the command, i.e. total dosed volume at the end of the command. Unit: mL
'**Volume.FP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the fixed point is reached. Unit: mL

In the case of variables with index **{x}**, the index **{1}** is set automatically at the time of insertion in a formula. This index can be set manually to 2–9 (e.g., '**Volume.EP{3}**.*Command name*' for the volume of the third equivalence point).

Equipment variables
'**Concentration.CurrentSolution**.*Command name*' Concentration of the solution used that is dosed with the dosing unit or buret (corresponds to the concentration of component 1 in the solution used). Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable
'**Diameter.AspirationTube.CurrentSolution**.*Command name*' Diameter of the aspiration tubing that is connected to the Liquid Adapter. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the Liquid Adapter. Unit: cm
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.

Equipment variables
'**Name.CurrentSolution**.*Command name*' Name of the solution used with the dosing unit.
'**Titer.CurrentSolution**.*Command name*' Titer of the solution connected to the Liquid Adapter that is dosed with the dosing unit. The titer is the factor that indicates the deviation of the actual concentration from the nominal concentration of a solution. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Concentration unit of the solution that is dosed with the dosing unit (corresponds to the concentration unit of component 1 in the solution). It is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer of the solution that is connected to the Liquid Adapter and that is dosed with the dosing unit.

See also

TET – Properties (chapter 5.11.8.5.1, page 501)

TET – Run (chapter 5.11.8.5.2, page 507)

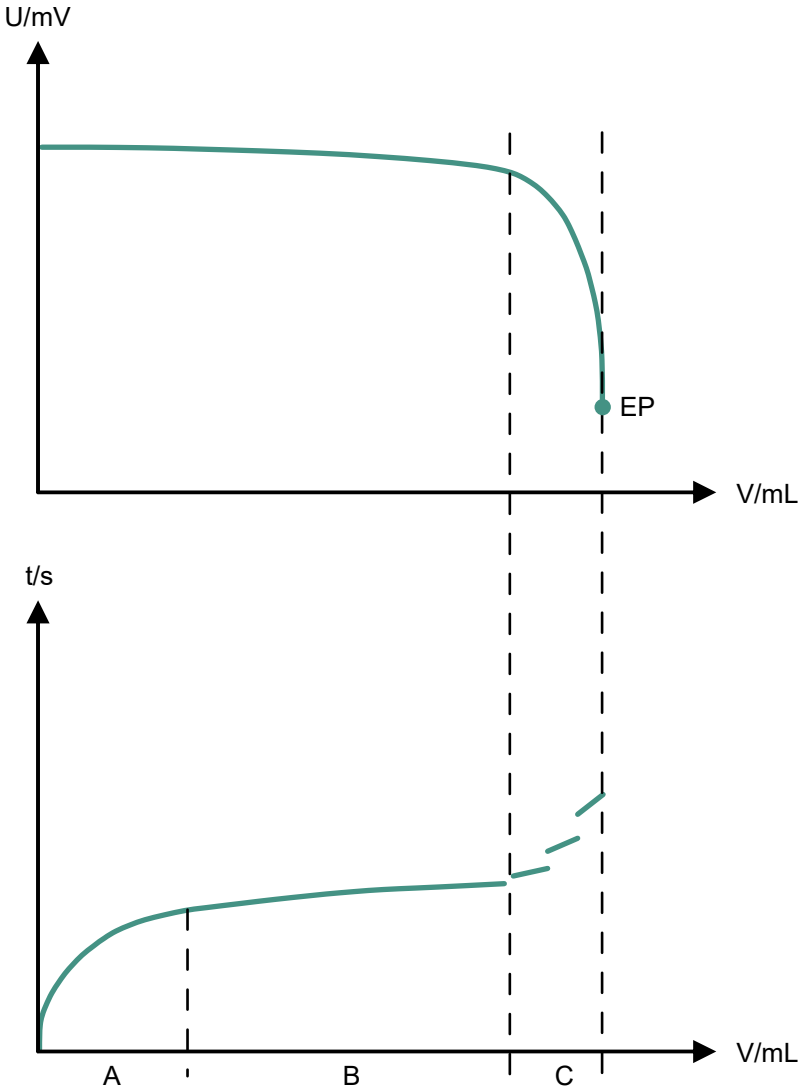
5.11.8.6 SET – Principle

Principle

The **SET** command is used to carry out titrations to one or two specified endpoints. The titration is canceled at the endpoint, either drift-controlled or after a waiting time which can be defined. The volume that has been dosed up to the endpoint gives the calculable reagent consumption.

The reagent is added in three phases during the titration:

- **Initial dosing**
  The dosing rate increases continuously during this phase. Initially, the dosing rate corresponds to the value of the **Minimum dosing rate** parameter . After that, the dosing rate is continuously increased until the value of the parameter **Maximum dosing rate** is reached.
- **Continuous dosing**
  During this phase, dosing is continuous until the **Control range** is reached. The dosing rate corresponds to the value for **Maximum dosing rate**.
- **Control range**
  The dosing rate is reduced as soon as the defined **Control range** is reached. The closer the endpoint, the slower the dosing in the control range. Shortly before the endpoint is reached, dosing is only still carried out at the value of the **Minimum dosing rate** parameter.



EP = Endpoint

A = Initial dosing

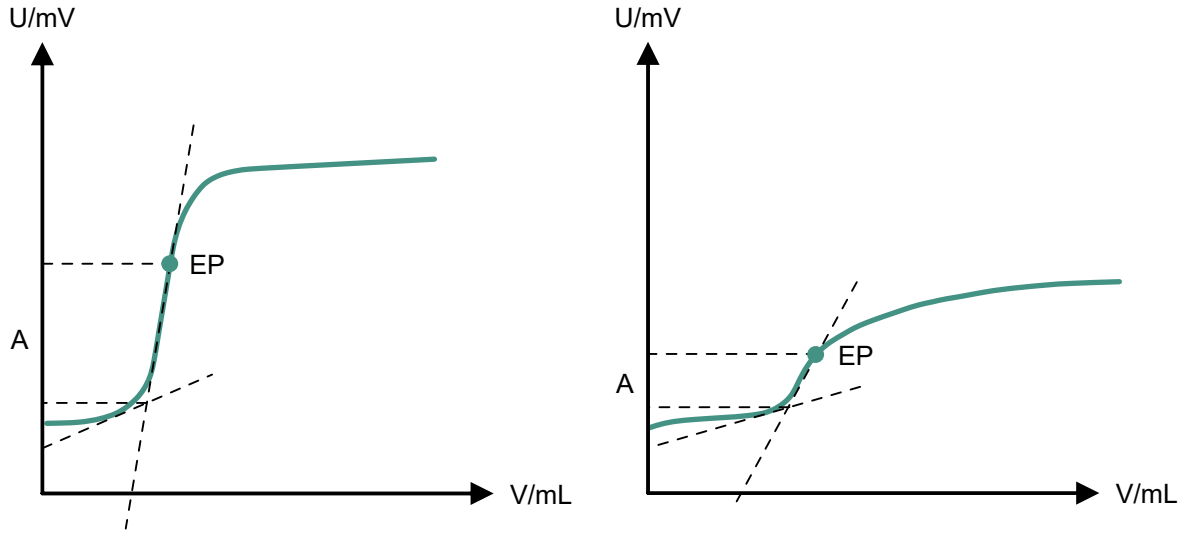
B = Continuous dosing

C = Control range

This command can be used for rapid routine determinations where the endpoint does not change throughout a series or for titrations where an excess of reagent must be avoided.

Control range

Set a large control range for steep curves and a small control range for flatter ones. A good approximation for the start of the control range is provided by the point where the tangents intersect.



EP = Endpoint

A = Control range

See also

SET – Command variables (chapter 5.11.8.6.3, page 530)

SET – Properties (chapter 5.11.8.6.1, page 512)

5.11.8.6.1 SET – Properties

The **SET** command is used to carry out endpoint titrations (**SET** = **S**et **E**ndpoint **T**itration).

Depending on the measured quantity required, the following commands can be selected:

- **SET Ipol**
  Endpoint titration with voltametric potential measurement with selectable polarization current (measured quantity: Potential U)
- **SET pH**
  Endpoint titration with potentiometric pH measurement (measured quantity: pH)
- **SET U**
  Endpoint titration with potentiometric potential measurement (measured quantity: Potential U)

The determination can be paused manually during the execution of a **SET** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped via the status menu.

After selecting a **SET** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are dis-

played: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the commands **SET Ipol**, **SET pH** and **SET U**:

Parameters

The **Parameters for conditioning** are only effective if the endpoint titration is carried out with conditioning. The **COND ON** and **COND CHECK** commands must be present in the process sequence before the **SET Ipol** command for this purpose.

Parameters for conditioning	
Start drift	The **Start drift** is a threshold value that the volume drift needs to be below during the entire **Stabilizing time** so that the **Conditioning OK** status is reached. The value should be adjusted to the titrant and humidity conditions.
Stabilizing time	The **Stabilizing time** starts as soon as the volume drift falls below the **Start drift**. If the volume drift has fallen below the **Start drift** during the entire **Stabilizing time**, then the status **Conditioning OK** is reached after the **Stabilizing time** has elapsed. As soon as the volume drift once again exceeds the **Start drift** during the **Stabilizing time**, the **Stabilizing time** is re-initialized. If an extraction method with oven is used for the water content determination, Metrohm recommends increasing the value to at least 10 s.
Sample addition time	The **Sample addition time** is a waiting time between the end of the conditioning and the start of the titration which is waited for before adding the sample into the titration cell.
Correction with volume drift	The correction volume is subtracted from the endpoint volume with the **Correction with volume drift** parameter. The use of the **Correction with volume drift** is displayed in the raw data. The following options can be selected: ▪ **Off**: The endpoint volume is not corrected. ▪ **Automatic**: The correction volume is calculated with the volume drift that was determined during conditioning. ▪ **Manual**: The correction volume is calculated with the following **Volume drift** parameter. The influx of humidity can cause a volume drift of up to 20 µL/min even with leakproof titration cells.

Parameters for conditioning	
Volume drift	The **Volume drift** parameter is only active if the **Correction with volume drift** was activated with **Manual**. Metrohm recommends determining the value of the volume drift in advance with a blind titration over several minutes with the equipment used.
Conditioning stop volume	If the **Conditioning stop volume** is reached during conditioning, the determination is canceled with a message as it has to be assumed that there is a problem. The conditioning stop volume must be adjusted to the volume of the titration vessel in order to prevent any overflow.
Conditioning stop time	If the **Conditioning stop time** is reached during conditioning, the determination is canceled with a message as it has to be assumed that there is a problem.

Start conditions	
Signal drift initial measured value	The initial measured value is applied as soon as the signal drift falls below the defined value or no later than after the maximum waiting time has expired. **Off** deactivates the drift control.
Minimum waiting time	If drift control is enabled, the initial measured value will not be applied until after the minimum waiting time has expired at the earliest, and the measurement will be aborted, even if it has already fallen below the **Signal drift initial measured value**.
Maximum waiting time	**Drift control enabled:** If the signal drift does not fall below a defined value before the maximum waiting time has expired, then the initial measured value is adopted after the maximum waiting time has expired, and the measurement is aborted. **Drift control disabled:** The initial measured value is adopted after the maximum waiting time has expired and the measurement is canceled.
Start volume	The titrant is added before the start of titration until the start volume is reached. The following stop conditions are checked while dosing the start volume: ▪ **Stop volume** ▪ **Stop time**

Start conditions	
Dosing rate start volume	Rate at which the start volume is dosed. If, in the **Equipment** work area, a **Maximum dosing rate** is defined for dosing port 1 of the functional unit used that is smaller than the **Dosing rate start volume**, then the maximum dosing rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Pause	Waiting time, e.g. for the measured value to stabilize after start or as reaction time after dosing a start volume. The pause follows at the end of all the start conditions.

Control parameters EP 1	
Endpoint at	Measured value for the first endpoint.
Titration rate	The titration rate can either be determined using 3 predefined parameter sets, or the values for the titration parameters can be defined individually. ▪ **Slow**: Parameter set for titrations for which the finest details are to be visible. This can, however, lead to an increase in noise, which may result in unwanted equivalence points. ▪ **Optimal**: Parameter set that has been optimized for the most common applications. ▪ **Fast**: Parameter set for not very critical, fast titrations. ▪ **Enter values**: The values for the titration parameters must be defined individually. If a predefined parameter set is selected for the titration rate, the following parameters are displayed but they cannot be edited: ▪ **Control range** ▪ **Maximum dosing rate** ▪ **Minimum dosing rate** The values used can be read in the corresponding parameters.

Control parameters EP 1	
Control range	In the control range, the rate of the titrant dosing is controlled using the difference between the predefined endpoint and the current measured value. This means that titration to the endpoint is slower in the control range. Outside the control range, the dosing rate is continuously increased until the **Maximum dosing rate** is reached. With **Unlimited**, the entire measuring range is considered as **Control range**. **Note**: The setting **Unlimited** is identical to the setting **Off** in previous Metrohm applications. This parameter influences the accuracy with which the endpoint is reached. The larger the control range, the longer the titration will take but the more accurately the endpoint is approached. The control range can be reduced if accuracy has a subordinated role and titration should be carried out faster.
Maximum dosing rate	Maximum rate of acceleration outside the control range. Depending on the measured value change, it may not be possible to reach the maximum dosing rate. If a smaller **Maximum dosing rate** is defined for dosing port 1 of the used functional unit in the **Equipment** work area, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Minimum dosing rate	Rate at which dosing is carried out at the very beginning of the titration and in the control range at the end of the titration. The smaller this rate, the slower the titration and the higher the accuracy.

Control parameters EP 1	
Stop criterion	Once the first endpoint has been reached, the procedure pauses after the final dosing while awaiting the selected stop criterion to be reached. After this, the endpoint is considered to have been reached. If a second endpoint has been defined, then the regulated sequence continues to this point, otherwise the titration is ended. The following stop criteria can be selected: ▪ **Stop drift**: Once the first endpoint has been reached and the volume drift falls below the defined **Stop drift**, the end point is applied. If a second endpoint has been defined, then the regulated sequence continues to this point, otherwise the titration is ended. ▪ **Delay time**: Once the first endpoint has been reached and the defined **Delay time** has passed, the endpoint is applied. If a second endpoint has been defined, then the regulated sequence continues to this point, otherwise the titration is ended. ▪ **Off**: The titration is canceled only by the stop conditions. No endpoint data is saved as raw data.

Control parameters EP 2	
Endpoint at	Measured value for the second endpoint. With **Off**, no titration to the second endpoint will be carried out. **Note**: If the endpoint titration is carried out with conditioning, then the titration to the second endpoint must be disabled with **Off**.
Titration rate	The titration rate can either be determined using 3 predefined parameter sets, or the values for the titration parameters can be defined individually. ▪ **Slow**: Parameter set for titrations for which the finest details are to be visible. This can, however, lead to an increase in noise, which may result in unwanted equivalence points. ▪ **Optimal**: Parameter set that has been optimized for the most common applications. ▪ **Fast**: Parameter set for not very critical, fast titrations. ▪ **Enter values**: The values for the titration parameters must be defined individually. If a predefined parameter set is selected for the titration rate, the following parameters are displayed but they cannot be edited: ▪ **Control range** ▪ **Maximum dosing rate** ▪ **Minimum dosing rate** The values used can be read in the corresponding parameters.

Control parameters EP 2	
Control range	In the control range, the rate of the titrant dosing is controlled using the difference between the predefined endpoint and the current measured value. This means that titration to the endpoint is slower in the control range. Outside the control range, the dosing rate is continuously increased until the **Maximum dosing rate** is reached. With **Unlimited**, the entire measuring range is considered as **Control range**. **Note**: The setting **Unlimited** is identical to the setting **Off** in previous Metrohm applications. This parameter influences the accuracy with which the endpoint is reached. The larger the control range, the longer the titration will take but the more accurately the endpoint is approached. The control range can be reduced if accuracy has a subordinated role and titration should be carried out faster.
Maximum dosing rate	Maximum rate of acceleration outside the control range. Depending on the measured value change, it may not be possible to reach the maximum dosing rate. If a smaller **Maximum dosing rate** is defined for dosing port 1 of the used functional unit in the **Equipment** work area, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Minimum dosing rate	Rate at which dosing is carried out at the very beginning of the titration and in the control range at the end of the titration. The smaller this rate, the slower the titration and the higher the accuracy.
Stop criterion	Once the second endpoint has been reached, the procedure pauses after the final dosing while awaiting the selected stop criterion to be reached. After this, the endpoint is considered to have been reached and the titration is stopped. The following stop criteria can be selected: ▪ **Stop drift** ▪ **Delay time** ▪ **Off** If the stop criterion is set to **Off**, then the titration is canceled only by the stop conditions. No endpoint data is saved as raw data.
Stop drift	Once the second endpoint has been reached and the volume drift falls below the defined **Stop drift**, the end point is applied and the titration is ended.

Control parameters EP 2	
Delay time	Once the second endpoint has been reached and the selected **Delay time** has passed, the endpoint is applied and the titration is ended.

Titration parameters	
Titration direction	Selection of the titration direction. If only one endpoint has been defined, the following applies: ▪ **Positive**: In the direction of positive measured value change ▪ **Negative**: In the direction of negative measured value change ▪ **Automatic**: The titration direction is calculated with the initial measured value and the set endpoint. If 2 endpoints have been set, then the titration direction has already been defined and the selected titration direction is ignored. Metrohm recommends specifying the titration direction. If the titration direction is specified, a message is shown if the actual titration direction does not correspond to the one specified.
Extraction time	During the **Extraction time**, no endpoint is applied and the titration is not ended, even if the endpoint and the stop criterion have already been reached. The extraction time starts from the moment all start conditions have been processed. It is advisable to enter an **Extraction time**, e.g. for the titration of sparingly soluble samples.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the titration, even if the time interval has not yet been reached.

Titration parameters	
I(pol) DC (only SET Ipol)	The polarization current **I(pol) DC** (Direct Current) is the current that is applied to the polarizable electrode during voltametric measurement. **Note**: For OMNIS instruments, Metrohm recommends entering the current in increments of 0.5 µA. For instruments of the **Titrando** type an increment of 0.5 µA **must** be observed. For instruments of the **855 Robotic Titrosampler** type an increment of 2.5 µA **must** be observed. The **Endpoint at** and the **Control range** may also need to be adjusted when the polarization current is changed.
Carry out electrode check (only SET Ipol)	The electrode check is carried out for polarizable electrodes during the transition from an inactive normal status to the titration. It checks within a few seconds whether an electrode is connected and whether no short circuit is present. If the titration with conditioning is executed, the electrode check is carried out during the transition from the inactive normal status to conditioning.
Filling rate	Rate at which the cylinder is filled. If, in the **Equipment** work area, a smaller **Maximum filling rate** is defined for the fill port for the functional unit used, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If air bubbles form during the aspiration of the solution, then the filling rate needs to be reduced accordingly so that the dosing drive it is not overloaded.
Stop conditions	
Stop volume	The titration is canceled as soon as the defined volume has been dosed since the start of the titration (including start conditions). The volume must be adjusted to the size of the titration vessel to prevent it from overflowing. In addition, the **Stop volume** should always be smaller than or equal to the cylinder volume to avoid refilling during the titration. **Off** disables this stop condition.
Stop time	The titration is canceled as soon as the defined time has elapsed since the start of the determination (including start conditions). **Off** disables this stop condition.

Fixed point evaluation	
Define fixed points	The subsection for defining the fixed points is opened. *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*
Specified quantity	Selection of the specified quantity for the calculation of the fixed point from the measuring point list: Only valid for **SET Ipol**: ▪ **Potential** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume. Only valid for **SET pH**: ▪ **pH** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified pH value. ▪ **Time** The values **pH**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **pH**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume. Only valid for **SET U**: ▪ **Potential** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume.
Fixed point at	Specified measured value for the calculation of the fixed point.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Potential** Only valid for **SET Ipol**. ▪ **pH** Only valid for **SET pH**. ▪ **Potential** Only valid for **SET U**. ▪ **Time** (default value), **Volume**, **Drift**, **Temperature**. Valid for all **SET** commands.

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Potential** Only valid for **SET Ipol**. ▪ **pH** Only valid for **SET pH**. ▪ **Potential** Only valid for **SET U**. ▪ **Time**, **Volume** (default value), **Drift**, **Temperature**. Valid for all **SET** commands.

Chart – y2-axis	
Display y2-axis	Display of a second y-axis for displaying another quantity as a curve. Activation of the y2-axis via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Potential** (default value) Only valid for **SET Ipol**. ▪ **pH** (default value) Only valid for **SET pH**. ▪ **Potential** (default value) Only valid for **SET U**. ▪ **Time**, **Volume**, **Drift**, **Temperature**. Valid for all **SET** commands.

Curve simulation	
Curve selection	Simulated curves can be used with OMNIS instruments to check the determination run. The titration sequence is defined by the set parameters. The simulation must be deactivated before analyzing real samples. Selection of the simulation curve: ▪ **None** (default value) No simulation curve (the curve simulation is deactivated). ▪ **Hydrochloric acid** Simulation curve of the titration of hydrochloric acid with caustic soda (titration curve with one equivalence point). ▪ **Citric acid** Simulation curve of the titration of citric acid with caustic soda (titration curve with 3 equivalence points).

The curve simulation cannot be used for instruments of the **Titrando** and **855 Robotic Titrosampler** type.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift initial measured value**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Dosing rate start volume**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Endpoint at**
  Minimum value: –1,200.0 mV
  Maximum value: 1,200.0 mV
- **Endpoint at pH**
  Minimum value: –13.000
  Maximum value: 20.000
- **Maximum dosing rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Minimum dosing rate**
  Minimum value: 0.01 µL/min
  Maximum value: 9,999.00 µL/min

- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s
- **I(pol) DC** (Titrando)
  Minimum value: –122.5 µA
  Maximum value: 122.5 µA
  Permitted increment: 0.5 µA
- **I(pol) DC** (855 Robotic Titrosampler)
  Minimum value: –122.5 µA
  Maximum value: 122.5 µA
  Permitted increment: 2.5 µA
- **Filling rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Fixed point at**
  Minimum value SET Ipol and SET U: –1,200.0 mV
  Maximum value SET Ipol and SET U: 1,200.0 mV
  Minimum value SET pH: –13.000
  Maximum value SET pH: 20.000

Execute with

In order for a **SET** command to be executed, the corresponding functional units and, for analog measuring inputs, the required sensor need to be assigned to the command.

- Dosing unit or buret to which the titrant is connected:
  Dosing Drive with connected **Cylinder Unit**, **800 Dosino** with connected **807 Dosing Unit**, **805 Dosimat** with connected **806 Exchange Unit** or **Internal Dosing Drive** with connected **806 Exchange Unit**
- Digital or analog measuring input to which the sensor required for titration is connected:
  Measuring Module Digital, **Measuring Module Analog**, **Measuring Interface iConnect**, **Measuring Interface Analog** or **Interface Coulometry**
- Sensor (digital, intelligent or analog):
  Polarizable metal electrode, **Ion-selective electrode**, **pH electrode**, **Metal electrode** or **Other sensor**

After a functional unit for the command has been selected, the following additional parameters appear:

For **Dosing Drive**:

Dosing port	Port that is to be used to dose a volume increment. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1 (default value). ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2.
For **Measuring Module Analog**:	
Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input (only for SET pH and SET U)	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **Difference**: Differential measurement between electrodes at INPUT 1 and INPUT 2.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties ► Parameters ► Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error. **Note**: For a combined pH/temperature sensor, both measuring inputs must be set to **INPUT 1**.
Measuring input (only for SET pH and SET U)	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.
For **Measuring Interface Analog** and **Measuring Interface iConnect** (SET pH and SET U):	

Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **Ind./Ref./Temp.**: Measurement with an analog electrode. ▪ **iConnect**: Measurement with an intelligent electrode (iTrode)
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Measuring Interface Analog** (SET Ipol):

Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: **Pol./Temp.**: Measurement with a polarizable electrode.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Interface Coulometry** (SET Ipol):

Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: **Ind./Temp.**: Measurement with an analog electrode and/or a temperature sensor.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

DET – Properties (chapter 5.11.8.3.1, page 445)

KFC – Properties (chapter 5.11.8.11, page 586)

KFT – Properties (chapter 5.11.8.10.1, page 568)

MET – Properties (chapter 5.11.8.4.1, page 472)

SET – Command variables (chapter 5.11.8.6.3, page 530)

SET – Principle (chapter 5.11.8.6, page 510)

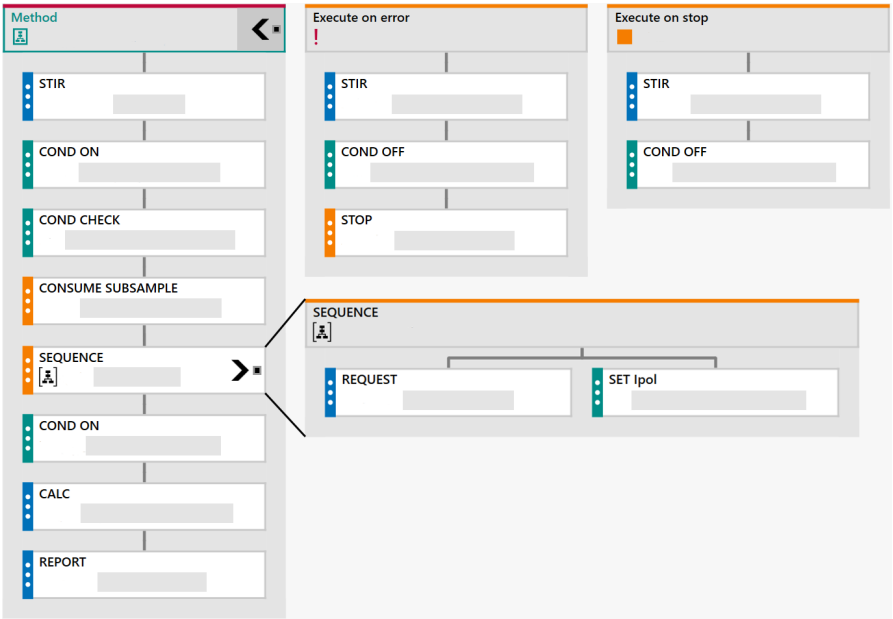
SET – Run (chapter 5.11.8.6.2, page 527)

Sensor – Definition (chapter 5.12.6, page 998)

5.11.8.6.2 SET – Run

The **SET Ipol** command can be executed with and without conditioning.
If conditioning is necessary, the conditioning commands **COND ON** (Start conditioning) and **COND CHECK** (Monitor conditioning) must be inserted before the **SET Ipol** command.
If reconditioning is necessary, a **COND ON** command must be inserted in the method again after the **SET Ipol** command.

A standard method for **SET Ipol** with conditioning may look as follows:



The **SET** command is executed in the following steps:

1 – Preconditioning

A **SET Ipol** work system can be conditioned by inserting a **COND ON** and a **COND CHECK** command before the **SET Ipol** command in the **SET Ipol** method.

The transition from conditioning to titration is defined in the **COND CHECK** command under **Titration start**. If **Manual** was selected, the titration can be started manually after conditioning with the **[Start titration]** button in the live data of the determination. If **Automatic after COND OK** was selected, the titration starts automatically as soon as the conditioning conditions **Start drift** and **Stabilizing time** of the referenced titration command are fulfilled and the **Sample addition time** has elapsed.

2 – Determining the initial measured value

The initial measured value (measured value before start of pre-dosing) is determined according to the parameters in the parameter group **Start conditions**, either drift-controlled or after a maximum waiting time has elapsed.

3 – Processing the start conditions

If a **Start volume** was defined in **Start conditions**, it is pre-dosed before the actual titration. The defined **Pause** time is then observed.

4 – Carrying out the titration

The titration is carried out according to the parameters defined under **Control parameters EP 1**, **Control parameters EP 2** and **Titration**

parameters. If a **SET Ipol** command is executed with conditioning, only 1 endpoint may be defined.

- **Fixed point evaluation**
  Optionally, up to 9 fixed points can be defined in **Fixed point evaluation** that are calculated from the measuring point list during the titration.
- **Graph – … axes**
  Optionally, different quantities can be selected for the x-axis and y-axis. In addition, a y2-axis can be displayed.

5 – Completing the titration

For titrations with 1 defined endpoint: The titration is completed as usual, as soon as the endpoint defined in **Control parameters EP 1** and the stop criterion are reached.

For titrations with 2 defined endpoints: The titration is completed as usual, as soon as the endpoints defined in **Control parameters EP 1** and **Control parameters EP 2** and the stop conditions are reached.

The conditions defined under **Stop conditions** are constantly monitored during the titration. By defining one or more stop conditions, the user makes sure that e.g. the titration vessel does not overflow if the endpoint is not reached or if the stop criterion is never met. The titration is canceled if one of these conditions applies.

A running titration can be canceled by a manual cancellation or with the emergency stop or in case of an error.

6 – Reconditioning

A **SET Ipol** work system can be conditioned further after the determination has ended (reconditioning) by inserting another **COND ON** command in the **SET Ipol** method at the end of a process sequence after a **SET Ipol** command.

In doing so, the titration cell is conditioned even without a running sub-sample. Conditioning can be stopped manually in the window of the respective work system.

See also

Conditioning – Principle (chapter 5.11.8.10, page 567)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

SET – Command variables (chapter 5.11.8.6.3, page 530)

SET – Principle (chapter 5.11.8.6, page 510)

SET – Properties (chapter 5.11.8.6.1, page 512)

5.11.8.6.3 SET – Command variables

The following variables are generated by the commands **SET pH**, **SET U** and **SET Ipol** in the process sequence and can be used in a formula under the designation '**Variable name**.*Command name*'.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Driftvalue.DriftCorrection**.*Command name*' (only SET Ipol with conditioning) Volume drift that was used for correcting the EP volume. When working with conditioning, this volume drift is used for calculating the EP volume correction if the **Correction with volume drift** parameter was activated (**Automatic** or **Manual**). Unit: µL/min
'**Driftvalue.EP{x}**.*Command name*' (x = 1–9) Volume drift of the endpoint. Unit: µL/min
'**Driftvalue.Final**.*Command name*' Volume drift for the last measuring point in the measuring point list. Unit: µL/min
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**Duration.DriftCorrection**.*Command name*' (only SET Ipol with conditioning) Period from the end of conditioning until the end of the titration. When working with conditioning, this time period is used for calculating the EP volume correction if the **Correction with volume drift** parameter was activated (**Automatic** or **Manual**). Unit: s
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

Command variables
'**Index.EP{x}**.*Command name*' (x = 1–9) Index of the endpoint. Unit: None
'**Index.FP{x}**.*Command name*' (x = 1–9) Index of the fixed point. Unit: None
'**Measvalue.EP{x}**.*Command name*' (x = 1–9) Measured value of the endpoint. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.FP{x}**.*Command name*' (x = 1–9) Measured value of the fixed point. Unit: None (SET pH) or mV (SET U, SET Ipol)
'**Temperature.EP{x}**.*Command name*' (x = 1–9) Temperature associated with the endpoint. Unit: °C
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Temperature.FP{x}**.*Command name*' (x = 1–9) Temperature associated with the fixed point. Unit: °C
'**Time.EP{x}**.*Command name*' (x = 1–9) Time stamp associated with the endpoint. Unit: s
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Time.FP{x}**.*Command name*' (x = 1–9) Time stamp associated with the fixed point. Unit: s

Command variables
'**Unit.Measvalue**.*Command name*' Unit of the measured values.
'**Volume.DriftCorrection**.*Command name*' (only SET Ipol with conditioning) Volume that was calculated for the drift-based correction of the EP volume. The correction volume is calculated by multiplying the volume drift with the period from the end of conditioning until the end of the titration. When working with conditioning, this volume is used for the EP volume correction if the **Correction with volume drift** parameter was activated (**Automatic** or **Manual**). Unit: mL
'**Volume.EP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the endpoint is reached. Unit: mL
'**Volume.Final**.*Command name*' End volume after processing the command, i.e. total dosed volume at the end of the command. Unit: mL
'**Volume.FP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the fixed point is reached. Unit: mL

In the case of variables with index **{x}**, the index **{1}** is set automatically at the time of insertion in a formula. This index can be set manually to a number from 2–9 (e.g. '**Volume.EP{2}**.*Command name*' for the volume of the second endpoint).

Equipment variables
'**Concentration.CurrentSolution**.*Command name*' Concentration of the solution used that is dosed with the dosing unit or buret (corresponds to the concentration of component 1 in the solution used). Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable
'**Diameter.AspirationTube.CurrentSolution**.*Command name*' Diameter of the aspiration tubing that is connected to the Liquid Adapter. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the Liquid Adapter. Unit: cm

Equipment variables
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.
'**Name.CurrentSolution**.*Command name*' Name of the solution used with the dosing unit.
'**Slope.CurrentSensor**.*Command name*' Quotient from the slope of the sensor used and the Nernst slope with the respective temperature. This variable is available only for pH electrodes and ion-selective electrodes. Unit: Depends on the selected sensor
'**Titer.CurrentSolution**.*Command name*' Titer of the solution connected to the Liquid Adapter that is dosed with the dosing unit. The titer is the factor that indicates the deviation of the actual concentration from the desired concentration of a titrant. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Concentration unit of the solution that is dosed with the dosing unit (corresponds to the concentration unit of component 1 in the solution). The unit is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer of the solution that is connected to the Liquid Adapter and that is dosed with the dosing unit.
'**ZeroPoint.CurrentSensor**.*Command name*' Electrode zero point of the sensor used. This variable is available only for pH electrodes and ion-selective electrodes. Unit: Determined by the sensor used.

See also

SET – Properties (chapter 5.11.8.6.1, page 512)

SET – Run (chapter 5.11.8.6.2, page 527)

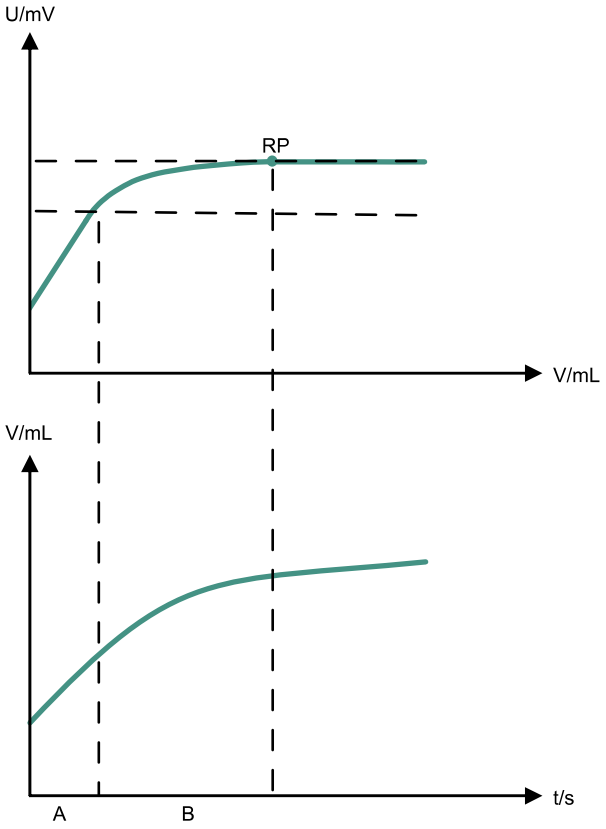
5.11.8.7 STAT – Principle

Principle

With the **STAT** command, a preset measured value (control point) can be reached and maintained at a constant level by adding a reagent. Because the substance that is released as a result of the reaction is at the same time titrated off again with the titrant, the controller must be able to maintain the preset control point at a constant level until the stop condition has been reached.

The reagent is added in 2 phases during titration:

- **Dosing outside the control range**
  The dosing rate increases continuously during this phase. Initially, the dosing rate corresponds to the value of the **Minimum dosing rate** parameter . After that, the dosing rate is continuously increased until the value of the parameter **Maximum dosing rate** is reached. The dosing continues to be carried out at the maximum rate until the control range is reached.
- **Dosing inside the control range**
  During this phase, the dosing rate is reduced until the control point is reached. Once this has been reached, the deviating measured values are compensated and the measured value is maintained at a constant level until the first stop condition has been met.



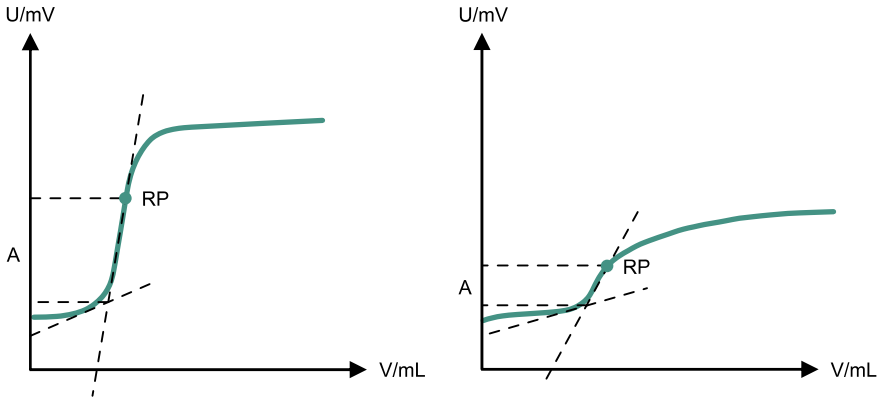
RP = Control point

A = Initial dosing

B = Control range

Control range

It is best to choose a large control range for steep curves and a small control range for flatter curves. A good approximation for the start of the control range is the point where the tangents intersect.



RP = Control point

A = Control range

Rate evaluation

The **EVAL LINEAR REGRESSION** command can be used for the rate evaluation with the **STAT** command. A linear regression is carried out in the same subsample over a defined measuring point range in the measuring point list. If the quantity **Time** is selected for the parameter **Quantity on the x-axis** and the quantity **Volume** is selected for the parameter **Quantity on the y-axis**, then the command variable '**Slope.Result**.*Command name*' outputs the rate.

Additional information on the **EVAL LINEAR REGRESSION** command:
(see "EVAL LINEAR REGRESSION – Parameters", chapter 5.11.8.68, page 776)

See also

Executing tandem dosing (chapter 5.12.3.14, page 939)

STAT – Command variables (chapter 5.11.8.7.3, page 544)

STAT – Properties (chapter 5.11.8.7.1, page 535)

STAT – Run (chapter 5.11.8.7.2, page 543)

5.11.8.7.1 STAT – Properties

The **STAT** command is used to carry out a titration where a preset measured value (control point) is reached and maintained at a constant level by adding a reagent.

Depending on the measured quantity required, the following commands can be selected:

- **STAT pH**
  Titration with a constant pH value.
- **STAT U**
  Titration with a constant potential.

The determination can be paused manually during the execution of a **STAT** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the commands **STAT pH**, and **STAT U**:

Parameters

Start conditions	
Signal drift initial measured value	The initial measured value is applied as soon as the signal drift falls below the defined value or no later than after the maximum waiting time has expired. **Off** deactivates the drift control.
Minimum waiting time	If drift control is activated, the initial measured value will not be applied until after the minimal waiting time has expired at the earliest, even if it has already fallen below the **Signal drift initial measured value**.
Maximum waiting time	**Drift control activated:** If the signal drift does not fall below a defined value before the maximum waiting time has expired, the initial measured value is adopted after the maximum waiting time has expired. **Drift control deactivated:** The initial measured value is adopted after the maximum waiting time has expired.
Start volume	The titrant is added before the start of titration until the start volume is reached. The following stop conditions are checked while dosing the start volume: ▪ **Stop volume** ▪ **Stop time**
Dosing rate start volume	Rate at which the start volume is dosed. If a smaller **Maximum dosing rate** is defined for dosing port 1 of the used functional unit in the **Equipment** work area, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.

Start conditions	
Pause	Waiting time, e.g. for the measured value to stabilize after start or as reaction time after dosing a start volume. The pause follows at the end of all the start conditions.

Control parameters	
Control point at pH (only STAT pH) **Control point at** (only STAT U)	Definition of the measured value to be controlled.
Titration rate	The titration rate can either be determined with 3 predefined parameter sets or the values for the titration parameters can be defined individually. ▪ **50 µL/min**: Parameter set for titrations with an expected reaction rate in the range of 50 µL/min. ▪ **100 µL/min**: Parameter set for titrations with an expected reaction rate in the range of 100 µL/min. ▪ **500 µL/min**: Parameter set for titrations with an expected reaction rate in the range of 500 µL/min. ▪ **Enter values**: The values for the titration parameters must be defined individually. If a predefined parameter set is selected for the titration rate, the following parameters are displayed but they cannot be edited: ▪ **Control range pH** or **Control range** ▪ **Maximum dosing rate** ▪ **Minimum dosing rate** The values used can be read in the corresponding parameters.
Control range pH (only STAT pH) **Control range** (only STAT U)	In the control range, the rate of the titrant dosing is controlled using the difference between the predefined control point and the current measured value. This means that titration to the control point is slower in the control range. Outside the control range, the dosing rate is continuously increased until the **Maximum dosing rate** is reached. With **Unlimited**, the entire measuring range is considered as **Control range**. ***Note***: The setting **Unlimited** is identical to the setting **Off** in previous Metrohm applications. This parameter influences the accuracy with which the control point is reached. The larger the control range, the longer the titration will take but the more accurately the control point is approached. The control range can be reduced if accuracy has a subordinated role and titration should be carried out faster.

Control parameters	
Maximum dosing rate	Maximum rate of acceleration outside the control range. Depending on the measured value change, it may not be possible to reach the maximum dosing rate. If a smaller **Maximum dosing rate** is defined for dosing port 1 of the used functional unit in the **Equipment** work area, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Minimum dosing rate	Rate at which dosing is carried out at the very beginning of the titration and in the control range at the end of the titration. The smaller this rate, the slower the titration and the higher the accuracy.

Titration parameters	
Titration direction	Selection of the titration direction. ▪ **Positive**: In the direction of positive measured value change ▪ **Negative**: In the direction of negative measured value change ▪ **Automatic**: The titration direction is calculated with the initial measured value and the set control point. Metrohm recommends specifying the titration direction.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the titration, even if the time interval has not yet been reached. **Note**: A titration with a **STAT** command can measure a maximum of 10,000 measuring points. The **Time interval measuring point** must be increased accordingly for long titrations.

Titration parameters	
Start time	The measuring points are not entered in the measuring point list until the specified period has elapsed since the start of the titration.
Start measured value pH (only STAT pH) **Start measured value** (only STAT U)	The measuring points are not entered in the measuring point list until the start measured value has been reached.
Filling rate	Rate at which the cylinder is filled. If, in the **Equipment** work area, a smaller **Maximum filling rate** is defined for the fill port for the functional unit used, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if air bubbles form during the aspiration of the solution, then the filling rate must be reduced accordingly so that the dosing drive is not overloaded.
Stop conditions	
Stop volume	The titration is canceled as soon as the defined volume has been dosed since the start of the titration (including start conditions). The volume must be adjusted to the size of the titration vessel to prevent it from overflowing. **Off** deactivates this stop condition.
Stop time criterion	Criterion to be used as a reference for the stop time and the cancellation of the titration: ▪ **Start**: The stop time starts as soon as all the start conditions have been processed. ▪ **Control point reached for first time**: The stop time starts as soon as the control point has been reached for the first time. ▪ **Last dosing**: The stop time starts after the last increment has been dosed, i.e., the stop time is reset to zero again after each dosing step. **Off** deactivates this stop condition. If a criterion is selected, the following specific parameter is displayed: ▪ **Period**
Period	The titration is canceled as soon as the defined period has elapsed since the selected stop time criterion occurred.

Stop conditions	
Stop rate	The titration is canceled as soon as the current dosing rate is lower than the stop rate defined here. ***Note***: This parameter is equivalent to the **Stop rate** parameter used in previous Metrohm applications with a modified input range. The numerical values from previous applications must be reduced by the factor 1000.

Fixed point evaluation	
Define fixed points	The subsection for defining the fixed points is opened. *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*
Specified quantity	Selection of the specified quantity for the calculation of the fixed point from the measuring point list: Only valid for **STAT pH**: ▪ **pH** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified pH value. ▪ **Time** The values **pH**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **pH**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume. Only valid for **STAT U**: ▪ **Potential** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume.
Fixed point at	Specified measured value for the calculation of the fixed point.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: Only valid for **STAT pH**: ▪ **pH** Only valid for **STAT U**: ▪ **Potential** Valid for all commands: ▪ **Time** (default value) ▪ **Volume** ▪ **Drift** ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: Only valid for **STAT pH**: ▪ **pH** Only valid for **STAT U**: ▪ **Potential** Valid for all commands: ▪ **Time** ▪ **Volume** (default value) ▪ **Drift** ▪ **Temperature**

Chart – y2-axis	
Display y2-axis	Display of a 2nd y-axis for representing another quantity as a curve. Activation of the y2-axis via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: Only valid for **STAT pH**: ▪ **pH** (default value) Only valid for **STAT U**: ▪ **Potential** (default value) Valid for all commands: ▪ **Time** ▪ **Volume** ▪ **Drift** ▪ **Temperature**

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Input ranges for parameters:

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, the corresponding input ranges have to be used for the following parameters:

- **Signal drift initial measured value**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Dosing rate start volume**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Control point at**
  Minimum value: –1,200.0 mV
  Maximum value: 1,200.0 mV
- **Control point at pH**
  Minimum value: –13.000
  Maximum value: 20.000
- **Maximum dosing rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Minimum dosing rate**
  Minimum value: 0.01 µL/min
  Maximum value: 9,999.00 µL/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s
- **Fixed point at**
  Minimum value STAT pH: –13.000
  Maximum value STAT pH: 20.000
  Minimum value STAT U: –1,200.0 mV
  Maximum value STAT U: 1,200.0 mV

Execute with

In order for a **STAT** command to be executed, the corresponding functional units and, for analog measuring inputs, the required sensor need to be assigned to the command.

- Dosing device to which the titrant is connected:
  800 Dosino with connected **807 Dosing Unit** or **805 Dosimat** with connected **806 Exchange Unit**

- Measuring input to which the sensor required for the titration is connected:
  Measuring Interface iConnect or **Measuring Interface Analog**
- Sensor (intelligent or analog):
  Polarizable metal electrode, **Ion-selective electrode**, **pH electrode**, **Metal electrode** or **Other sensor**

After a functional unit for the command has been selected, the following additional parameters appear:

Tandem dosing	If this check box is activated, uninterrupted dosing with 2 dosing devices combined takes place. While a dosing device is being filled, the dosing is carried out by the other dosing device. A secondary dosing device must be assigned to do this. Additional information on tandem dosing: *(see "Executing tandem dosing", chapter 5.12.3.14, page 939)*

See also

STAT – Command variables (chapter 5.11.8.7.3, page 544)

STAT – Principle (chapter 5.11.8.7, page 533)

STAT – Run (chapter 5.11.8.7.2, page 543)

5.11.8.7.2 STAT – Run

The **STAT** command is executed in 4 steps:

1 – Determining the initial measured value

The initial measured value (measured value before start of pre-dosing) is taken over either drift-controlled or after a maximum waiting time has elapsed.

2 – Processing the start conditions

If a **Start volume** was defined in **Start conditions**, it is pre-dosed before the actual titration. The defined **Pause** time is then observed.

3 – Carrying out the titration

The titration is carried out according to the parameters defined under **Control parameters** and **Titration parameters**.

- **Fixed point evaluation**
  Optionally, up to 9 fixed points can be defined in **Fixed point evaluation** that are calculated from the measuring point list during the titration.
- **Chart – … axes**
  Optionally, different quantities can be selected for the x-axis and y-axis. In addition, a y2-axis can be displayed.

A titration with a **STAT** command can measure a maximum of 10,000 measuring points. The **Time interval measuring point** must be increased accordingly for long titrations.

4 – Completing the titration

The titration is completed as usual as soon as the first stop condition defined in **Stop conditions** is fulfilled.

A running titration can be canceled by a manual cancellation or with the emergency stop or in case of an error.

See also

STAT – Command variables (chapter 5.11.8.7.3, page 544)

STAT – Principle (chapter 5.11.8.7, page 533)

STAT – Properties (chapter 5.11.8.7.1, page 535)

5.11.8.7.3 STAT – Command variables

The following variables are generated by the commands **STAT pH** and **STAT U** in the process sequence and can be used in a formula under the designation '**Variable name**.*Command name*'.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Driftvalue.Final**.*Command name*' Drift for the last measuring point in the measuring point list. Unit: dV/dt
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

Command variables
'**Index.FP{x}**.*Command name*' (x = 1–9) Index of the fixed point. Unit: None
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**' variable
'**Measvalue.FP{x}**.*Command name*' (x = 1–9) Measured value of the fixed point. Unit: Defined in the '**Unit.Measvalue**' variable
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Temperature.FP{x}**.*Command name*' (x = 1–9) Temperature associated with the fixed point. Unit: °C
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. This variable is available only for OMNIS instruments. Unit: s
'**Time.FP{x}**.*Command name*' (x = 1–9) Time stamp associated with the fixed point. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of the measured values.
'**Volume.Final**.*Command name*' End volume after processing the command, i.e. total dosed volume at the end of the command. Unit: mL
'**Volume.FP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the fixed point is reached. Unit: mL

In the case of variables with index **{x}**, the index **{1}** is set automatically at the time of insertion in a formula. This index can be set manually to a number from 2–9 (e.g. '**Volume.FP{3}**.*Command name*' for the volume of the third endpoint).

Equipment variables
'**Concentration.CurrentSolution**.*Command name*' Concentration of the solution used that is dosed with the dosing device (corresponds to the concentration of component 1 in the solution used). Unit: Defined in the '**Unit.Concentration.CurrentSolution**' variable
'**Diameter.AspirationTube.CurrentSolution**.*Command name*' Diameter of the aspiration tubing that is connected. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected. Unit: cm
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.
'**Name.CurrentSolution**.*Command name*' Name of the solution used with the dosing device.
'**Slope.CurrentSensor**.*Command name*' Quotient from the slope of the sensor used and the Nernst slope with the respective temperature. This variable is available only for pH electrodes and ion-selective electrodes. Unit: Depends on the selected sensor
'**Titer.CurrentSolution**.*Command name*' Titer of the connected solution that is dosed with the dosing device. The titer is the factor that indicates the deviation of the actual concentration from the desired concentration of a titrant. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Concentration unit of the solution that is dosed with the dosing device (corresponds to the concentration unit of component 1 in the solution). The unit is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer of the connected solution that is dosed with the dosing device.
'**ZeroPoint.CurrentSensor**.*Command name*' Electrode zero point of the sensor used. This variable is available only for pH electrodes and ion-selective electrodes. Unit: Determined by the sensor used.

See also

STAT – Principle (chapter 5.11.8.7, page 533)

STAT – Properties (chapter 5.11.8.7.1, page 535)

STAT – Run (chapter 5.11.8.7.2, page 543)

5.11.8.8 STDADD ISE – Principle

Principle

The commands **STDADD ISE auto** and **STDADD ISE dos** are used to perform a standard addition with an ion-selective electrode. For this, a known amount of the substance to be determined is added to the sub-sample either once or several times. The volumes to be added are either predefined or variable (so that a constant, defined potential difference can be reached).

As opposed to direct ion measurement with ion-selective electrodes, the ions of interest and interfering ions cannot be distinguished in the standard addition procedure, as both are present in the sample at the beginning. Only the sum can be determined. Therefore, a linear correlation between the measuring voltage U_i and the logarithm of the ion concentration to be determined c_i is generally assumed for standard addition measurements.

$$U_i = E(0) + \frac{U_N}{z} \cdot \log(c_i)$$

The regression line (linear regression) is thus determined iteratively according to the method of least squares. This procedure provides the axis intercept $E(0)$, the slope s and the concentration of the measuring ion in the diluted measuring solution c_A.

$$c_A = 10^{\frac{U_A - E(0)}{s}}$$

The dilution is taken into account via the parameters **sample volume** V_S (sample size in mL) and **volume auxiliary solution** V_{Add}, so that the end result c_S (concentration of the ion searched in the sample solution) can be calculated and directly displayed as follows:

$$c_s = \frac{V_s + V_{Add}}{V_s} c_A$$

The **STDADD ISE auto** and **STDADD ISE dos** commands can be used for the following instruments with the corresponding license: **OMNIS Titrator**, **OMNIS Titration Module**, **867 pH Module**, **904 Titrando**, **905 Titrando**, **906 Titrando** and **907 Titrando**.

Recalculating the values for the axis intercept $E(0)$, the slope s and the concentration c_A iteratively from the voltages U_i measured for the sample and the spiked solutions as well the known concentration of the standard solution requires much effort, because it is an equation system with 3 unknowns. However, the concentration c_S can at least be easily recalculated with the calculated values for $E(0)$, U_S and s (see the following example).

Example

- **Parameters**
  Concentration of the standard addition solution = 1,000 ppm
  Volume of the standard addition solution V_{add} = 10 mL
  Sample size V_S = 10 mL
- **Measured data**

	dV / mL	U / mV	dU / mV
Sample		59.8	
Increment 1	0.310	39.9	–20.0
Increment 2	0.705	19.9	–20.0
Increment 3	1.750	–1.1	–21.0

- **Result**
  $E(0)$ = 129.7 mV
  s = –61.5 mV
  $c(F^-)$ = **27.4 ppm**
- **Recalculation**
  c_A = 10^((59.8 – 129.7) / –61.5) = 13.696 ppm
  $c(F^-)$ = (10 + 10) / 10 * 13.696 = **27.39 ppm**

Recommendation

In order to guarantee a reliable evaluation of the standard addition, take care to ensure that the buret volume and the concentration of the standard solution are adjusted to the respective measuring conditions. The individual addition volumes must be selected in such a way that the potential difference is at least 12 mV after each additive step. The determination is canceled if the potential difference between 2 measurements is below 6 mV. A minimum of 4 volume increments should be dosed.

Recommended concentrations of the standard solution for the standard addition:

Buret volume / mL	$c_{Standard\ solution}$ / c_{Sample}
5	40 : 1
10	20 : 1

20	10 : 1
50	5 : 1

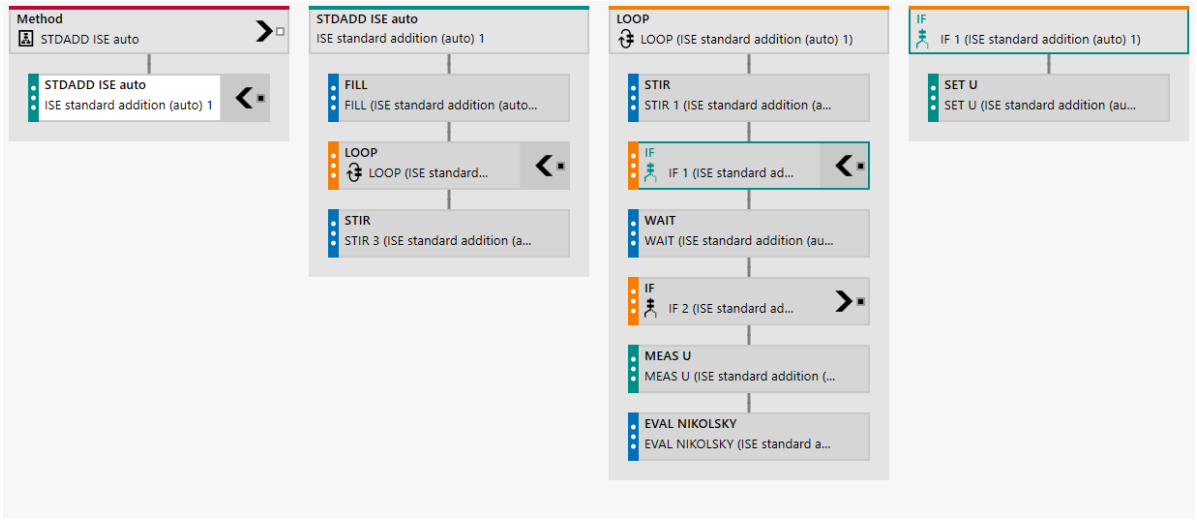
Example of a standard addition

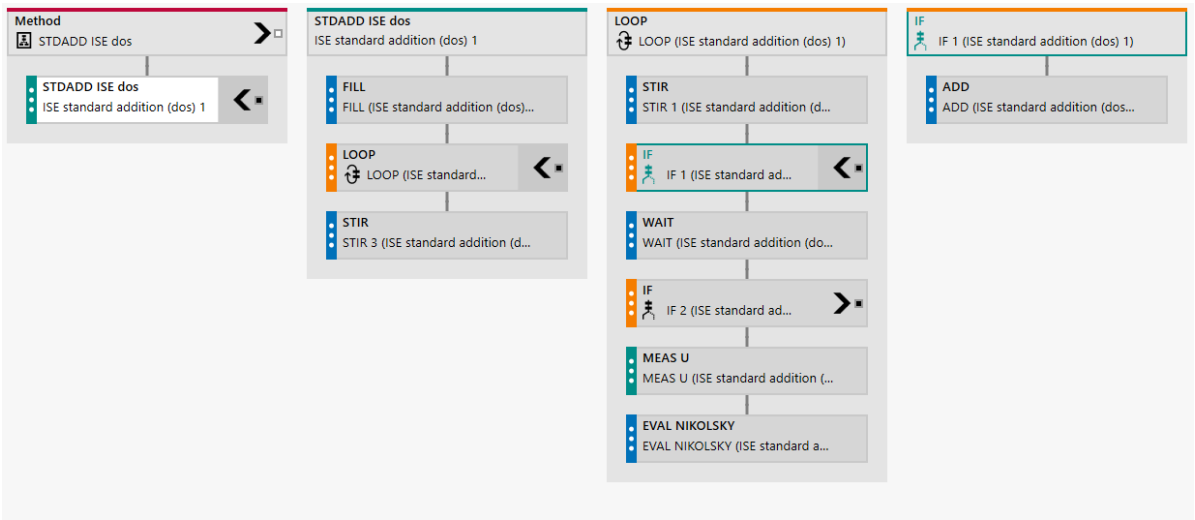
This example is valid for standard additions with any type of ion-selective electrodes.

Sample concentration	5 mg/L
Buret volume	10 mL
Sample size	10 mL
ISA/TISAB	10 mL
Total volume	20 mL
Factor $c_{Standard\ solution}/c_{Sample}$	20

This results in a sample concentration in the measuring solution of 2.5 mg/L. The optimum concentration of the standard solution is thus 2.5 mg/L · 20 = 50 mg/L. Please note that this is merely to be considered a guideline for standard additions. Even in case of deviations from this recommendation, precise measurements will still be possible.

Representation and structure





A non-modifiable sequence of individual commands is executed for the commands **STDADD ISE auto** and **STDADD ISE dos**. Clicking on ❯ displays the sequence in a separate area. Clicking ❮ closes the separate area again.

The commands contained within are not parameterized separately, but in the corresponding **STDADD ISE auto** command or **STDADD ISE dos** command. Moreover, the functional units for all the commands are selected in the **Execute with** subsection of the corresponding **STDADD ISE auto** command or **STDADD ISE dos** command.

Further information about the commands contained in **STDADD ISE auto** and **STDADD ISE dos**: *(see "STDADD ISE – Run", chapter 5.11.8.8.2, page 557)*

In the areas in the OMNIS Software, where values and results of a command are displayed (e.g. under **Subsample** ▶ **History** or under **Curves and data** ▶ **Live data**) all the commands contained in **STDADD ISE auto** and **STDADD ISE dos** are listed.
The results and curves of all commands are also output in the reports, except for in the short reports **Sample result report (short)** and **Subsample result report (short)**. Only the results and the curve of the standard addition is output there.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

STDADD ISE – Command variables (chapter 5.11.8.8.3, page 558)

STDADD ISE – Properties (chapter 5.11.8.8.1, page 551)

STDADD ISE – Run (chapter 5.11.8.8.2, page 557)

5.11.8.8.1 STDADD ISE – Properties

The commands **STDADD ISE auto** and **STDADD ISE dos** are used to execute standard additions with an ion-selective electrode. Depending on the procedure required, the following commands can be selected:

- **STDADD ISE auto**
  Determination of the ion concentration in a solution with an ion-selective electrode by automatically adding standard solution in order to reach a defined, constant potential difference. The required volume increments are calculated automatically.
- **STDADD ISE dos**
  Determination of the ion concentration in a solution with an ion-selective electrode by adding defined volume increments.

The determination can be paused manually during the execution of a **STDADD ISE** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped via the status menu.

After selecting a **STDADD ISE** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the commands **STDADD ISE auto**, and **STDADD ISE dos**:

Parameters

Standard addition parameters	
Sample volume	Volume of the sample.
Auxiliary solution volume	Volume of all auxiliary solutions that are added to the sample.
Number of additions (only STDADD ISE auto)	Number of additions of volume increments of the standard solution. We recommend a minimum of 4 additions.
Delta U (only STDADD ISE auto)	Potential difference that is to be reached per volume increment.
Define volume increments (only STDADD ISE dos)	The subsection for defining volume increments is opened. Here, between 1 and 19 volume increments can be defined. We recommend a minimum of 4 volume increments.

Standard addition parameters	
Dosing rate	Rate at which the volume increments are dosed. The rate can be configured freely for the **STDADD ISE dos** command. The rate can be selected with the **STDADD ISE auto** command: ▪ **Slow** Control range: 300 mV Maximum dosing rate: 1 mL/min Minimum dosing rate: 5 µL/min ▪ **Medium** Control range: 100 mV Maximum dosing rate: 10 mL/min Minimum dosing rate: 25µL/min ▪ **Fast** Control range: 30 mV Maximum dosing rate: maximum permitted rate for the dosing unit and buret used. Minimum dosing rate: 50µL/min
Filling rate	Rate at which the dosing unit is filled.
Stop volume (only STDADD ISE auto)	As soon as the sum of the dosed volume increments exceeds the volume defined here, the determination is canceled. To avoid having to fill during the addition, Metrohm recommends setting the stop volume to the same value as the volume of the buret used.
Stirring time before measurement	Stirring time between the addition of standard solution and the measurement in order to ensure the solution is mixed well. If the **Switch off stirrer during measurement** option is selected, the stirrer is switched off after the waiting time.

Measuring parameters	
Measuring method	Selection of the measuring mode. If **Drift-controlled measurement** is selected, the following specific parameters are displayed: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** If **Time-controlled measurement** is selected, the following specific parameter is displayed: ▪ **Measurement duration**
Signal drift	The measured value is applied as soon as the signal drift drops below the defined value.

Measuring parameters	
Minimum waiting time	If drift control is enabled, the measured value will not be applied until after the minimum waiting time has expired at the earliest, and the measurement is aborted, even if the signal drift has already fallen below a defined value. **Note**: This parameter corresponds to the sum of the **Pause before measurement** and **Minimum waiting time** parameters used in earlier Metrohm applications. The numerical values can be applied here if the subsample is not to be stirred for some time before the measurement.
Maximum waiting time	If drift control is enabled, the measured value is applied after the maximum waiting time has expired at the latest and the measurement is aborted, even if the signal drift has not yet been reached.
Measurement duration	For time-controlled measurements, the measurement is aborted as soon as the entered measurement duration is reached.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the time interval has not yet been reached.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the measuring solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously. If the temperature is measured with a temperature sensor, then the temperature determined at the first measurement will automatically be adopted as the reference temperature. The determination will be canceled with an error message if the temperature recorded during one of the subsequent measurements deviates by more than 2 °C from the reference temperature.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected.
Stirring parameters	
Stirring rate	Stirring rate (stirring level) and rotation direction of the stirrer. The following values can be entered: ▪ **+1** to **+15**: Stirring levels if the rotation direction of the solution is counterclockwise. ▪ **–1** to **–15**: Stirring levels when the rotation direction of the solution is clockwise.

Stirring parameters	
Switch off stirrer during measurement	If this check box is activated, the stirrer is switched off during the measurement.

The stirrer will be switched off automatically once the **STDADD ISE auto** command or the **STDADD ISE dos** command have finished. If the stirrer is to continue after the **STDADD ISE auto** command or the **STDADD ISE dos** command have finished, a **STIR** command must be added to the method.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Delta U** (STDADD ISE auto)
  Minimum value: 6.0 mV
  Maximum value: 999.0 mV
- **Dosing rate** (STDADD ISE dos)
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Filling rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min (800 Dosino)
  Maximum value: 150.00 mL/min (805 Dosimat, Internal Dosing Drive)
- **Signal drift**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s

Execute with

In order for a **STDADD ISE auto** command or a **STDADD ISE dos** command to be executed, the corresponding functional units and, for analog measuring inputs, the required sensor need to be assigned to the command.

- Dosing unit or buret to which the standard solution that was used is connected:
  Dosing Drive with connected **Cylinder Unit**, **800 Dosino** with connected **807 Dosing Unit**, **805 Dosimat** with connected **806 Exchange Unit** or **Internal Dosing Drive** with connected **806 Exchange Unit**
- Digital or analog measuring input to which the required sensor is connected:
  Measuring Module Digital, **Measuring Module Analog** or **Measuring Interface Analog**
- Sensor (digital or analog):
  Ion-selective electrode
- Stirrer:
  Magnetic Stirrer, **OMNIS Rod Stirrer**, **801 Stirrer**, **803 Ti Stand** or **804 Ti Stand**

After a functional unit for the command has been selected, the following additional parameters appear:

For **Dosing Drive**:	
Dosing port	Port that is to be used to dose a volume. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1 (default value). ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2.

For **Measuring Module Analog**:	
Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **Difference**: Differential measurement between electrodes at INPUT 1 and INPUT 2.

Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error. **Note**: For a combined pH/temperature sensor, both measuring inputs must be set to **INPUT 1**.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.

For **Measuring Interface Analog** and **Measuring Interface iConnect**:	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **Ind./Ref./Temp.**: Measurement with an analog electrode. ▪ **iConnect**: Measurement with an intelligent electrode (iTrode)
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

STDADD ISE – Command variables (chapter 5.11.8.8.3, page 558)

STDADD ISE – Principle (chapter 5.11.8.8, page 547)

STDADD ISE – Run (chapter 5.11.8.8.2, page 557)

5.11.8.8.2 STDADD ISE – Run

A non-modifiable sequence of individual commands is executed for the commands **STDADD ISE auto** and **STDADD ISE dos**:

1 – Filling

The **FILL** command is used for filling the cylinder with the standard solution connected to the functional unit.

The cylinder is only filled once at the beginning of the determination. No filling takes place between the steps for the addition and at the end of the determination.

2 – Determining the initial measured value

The initial measured values for the voltage and temperature are determined. The measured value acceptance either occurs drift-controlled or time-controlled via a **MEAS U** command, depending on the parameters set in the **Measuring parameters** parameter group.

3 – Addition

A volume increment of the standard solution is added.

- With the **STDADD ISE auto** command, standard solution is added via a **SET U** command until a defined potential difference is reached. With this, the volume increment can be calculated.
- With the **STDADD ISE auto** command, the volume increments entered in **Define volume increments** are added via an **ADD** command.

3 - Waiting time

In order to achieve a better mixing of the solution, a defined waiting time can be set during which the solution is still being stirred after the addition. This is executed via a **WAIT** command according to the parameters set in the **Standard addition parameters** parameter group.

4 - Measurement

The measured values for the voltage and temperature are determined after the addition. This is executed via a **MEAS U** command according to the parameters set in the **Measuring parameters** parameter group.

5 – Evaluation

The measured values are evaluated using the Nikolsky equation. This determines the concentration of the solution after adding each of the volume increments. The concentration of the sample and other values are calculated from the linear regression of the standard addition curve. This is executed via an **EVAL NIKOLSKY** command according to the parameters set in the **Standard addition parameters** parameter group.

6 – End the standard addition

Steps 2 to 5 are repeated for every volume increment in a **LOOP** command. Once all the steps for the addition have been executed, the standard addition is ended.

As the values are measured after each volume increment and the evaluation is done iteratively, the measured data is up to date at all times. If the standard addition is canceled because of an error, the interim results are available as variables.

The stirrer is controlled at various steps in the run via a **STIR** command according to the parameters set in the **Stirring parameters** parameter group.

See also

STDADD ISE – Command variables (chapter 5.11.8.8.3, page 558)

STDADD ISE – Principle (chapter 5.11.8.8, page 547)

STDADD ISE – Properties (chapter 5.11.8.8.1, page 551)

5.11.8.8.3 STDADD ISE – Command variables

The following variables are generated by the commands **STDADD ISE auto** and **STDADD ISE dos** in the process sequence and can be used in a formula as '**Variable name**.*Command name*'.

The variables available are stored in the **Command variables** and **Equipment variables** variable categories.

In the command variables, the variables of the **EVAL NIKOLSKY** command can be accessed. This command is not available in the command library, but is only used in the standard addition for evaluating the measured values using the Nikolsky equation.

While the variables of the commands **STDADD ISE auto** and **STDADD ISE dos** always display the measured values of the last run, the measured values for each individual volume increment can be checked via the **EVAL NIKOLSKY** variables. The number in the curly brackets is the number of the volume increment plus 1, because the first run of commands is executed without an addition.

Command variables

'**IntermediateSampleConcentration.Result**.*Command name*'

Intermediate result for the sample concentration resulting from the evaluation of the standard addition according to the Nikolsky equation. This corresponds to the concentration of the sample before the first addition and may be diluted by the auxiliary solution.

This variable is also available specifically for the **EVAL NIKOLSKY** command: '**IntermediateSampleConcentration.Result.**EVAL NIKOLSKY (*Command name*){}'

Unit: Corresponds to the concentration unit, set in the variable '**Unit.Concentration.StandardSolution**.*Command name*'

'**CoefficientOfDetermination.Result**.*Command name*'

The coefficient of determination (R^2) as a quality criterion of linear regression. The coefficient of determination indicates how suitable the independent variables are for explaining the variance of the dependent variables.

This variable is also available specifically for the **EVAL NIKOLSKY** command: '**CoefficientOfDetermination.Result**.EVAL NIKOLSKY (*Command name*){}'

Unit: None

'**Concentration.StandardSolution**.*Command name*'

Concentration of the standard solution used for the additions.

This variable is also available specifically for the **EVAL NIKOLSKY** command: '**Concentration.StandardSolution**.EVAL NIKOLSKY (*Command name*){}'

Unit: Set in the variable '**Unit.Concentration.StandardSolution.***Command name*'

'**DeltaU.Parameter**.*Command name*'

Potential difference defined by the user in **Standard addition parameters** that is to be reached per volume increment. This variable is only available for the **STDADD ISE auto** command.

Unit: mV

'**DosingVolume{}.Parameter**.*Command name*'

Volume increments in each step of the addition defined by the user in **Standard addition parameters**. The number in the curly brackets is the number of the volume increment. This variable is only available for the **STDADD ISE dos** command.

Unit: mL

'**Duration**.*Command name*'

Total duration for the processing of the command.

Unit: s

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**SampleConcentration.Result**.*Command name*'

The ion concentration of the undiluted initial sample calculated with the standard addition. In contrast to the variable '**IntermediateSampleConcentration.Result**.*Command name*', the dilution by the auxiliary solution is subtracted here.

This variable is also available specifically for the **EVAL NIKOLSKY** command: '**SampleConcentration.Result**.EVAL NIKOLSKY (*Command name*){}'

Unit: Corresponds to the concentration unit, set in the variable '**Unit.Concentration.StandardSolution.***Command name*'

'**Slope.Result**.*Command name*'

Electrode slope of the sensor used calculated with the standard addition.

This variable is also available specifically for the **EVAL NIKOLSKY** command: '**Slope.Result**.EVAL NIKOLSKY (*Command name*){}'

Unit: mV

'**StopVolume.Parameter**.*Command name*'

Stop volume defined by the user in **Standard addition parameters**. As soon as the sum of the dosed volume increments exceeds the stop volume, the determination is canceled. This variable is only available for the **STDADD ISE auto** command.

Unit: mL

'**TotalAddedVolume**.*Command name*'

Sum of all the volume increments that were dosed for the standard addition.

This variable is also available specifically for the **EVAL NIKOLSKY** command: '**TotalAddedVolume.Result**.EVAL NIKOLSKY (*Command name*){}'

Unit: mL

'**Unit.Concentration.StandardSolution**.*Command name*'

Unit of the concentration of the standard solution that was used for the volume increments.

This variable is also available specifically for the **EVAL NIKOLSKY** command: '**Unit.Concentration.StandardSolution**.EVAL NIKOLSKY (*Command name*){}'

'**Variance.Result**.*Command name*'

Measured value variance of the series. The variance is a measure for the dispersion of the data.

This variable is also available specifically for the **EVAL NIKOLSKY** command: '**Variance.Result**.EVAL NIKOLSKY (*Command name*){}'

Unit: None

'**ZeroPoint.Result**.*Command name*'

The electrode zero point of the sensor used calculated from the standard addition.

This variable is also available specifically for the **EVAL NIKOLSKY** command: '**ZeroPoint.Result**.EVAL NIKOLSKY (*Command name*){}'

Unit: mV

Equipment variables

'**Name.CurrentSensor**.*Command name*'

Name of the sensor used to measure the required measured quantity.

See also

STDADD ISE – Principle (chapter 5.11.8.8, page 547)

STDADD ISE – Properties (chapter 5.11.8.8.1, page 551)

STDADD ISE – Run (chapter 5.11.8.8.2, page 557)

5.11.8.9 Karl Fischer titration – Principle

Karl Fischer titration

The Karl Fischer titration is a procedure for water content determination.

When an aqueous sample is titrated with iodine in the presence of sulfur dioxide in a buffered, alcoholic solution, then several reactions take place that can be summarized in the following sum equation:

$H_2O + I_2 + [RNH]SO_3CH_3 + 2\ RN \Leftrightarrow [RNH]SO_4CH_3 + 2\ [RNH]I$

According to the equation above, the I_2 reacts quantitatively with H_2O.

This chemical equation serves as a basis for the water content determination.

Free as well as bound water can be determined using KF titration. Various procedures are used, depending on the quantity of the water content to be detected:

- **Volumetry**
  Water content levels of between 0.1 and 100% are preferred for volumetric titration.

- **Coulometry**
  Lower water content levels are preferred for coulometric titration. The determination range lies between 10 µg and 200 mg of water. Higher water content levels require a lot of time and/or might exceed the water capacity of the KF reagent, which can lead to faulty results.

The water content determination is carried out quickly and quantitatively in water-free solvents.

KF titration can be ended drift-controlled or once a defined delay time has elapsed. It determines the iodine consumption for the sample that is needed to calculate the water content.

Prerequisites for the KF titration

- The titration cell must be as leakproof as possible. As little moisture as possible should leak into the cell from the surrounding air.
- It must be possible to dose or generate the iodine as accurately as possible.
- No side reactions may occur.

Principle of the volumetric KF titration

When executing a volumetric Karl Fischer titration, an alcoholic solution of iodine, sulfur dioxide and a base as buffer substance is used.

The endpoint indication is effected voltametrically (Ipol) by modulating a direct current of constant strength to a double Pt electrode. This results in a potential difference at the double Pt electrode. It is drastically reduced as soon as even the slightest amounts of free iodine are present. This circumstance is used for detecting the endpoint of the titration.

Volumetry offers the advantages that solid as well as pasty samples can be introduced directly into the titration vessel and that the solution properties of the KF reagent can be tailored to the sample with a large number of suitable organic solvents. The volumetric KF reagents are not titration-stable, i.e. a regular titer determination is necessary for accurate results.

2 different types of KF reagents can be used:

- 1-component reagents: The titrant contains all of the reactants required for the KF reaction. The most commonly used solvent is dry methanol.
  Advantage: Greatest flexibility when selecting a sample-specific solvent. The required solvent is selected according to the characteristics regarding chemical composition and solubility of the sample to be analyzed. Unlimited water capacity.
  Disadvantage: Lacking titer stability. The titer continuously needs to be redetermined.

- 2-component reagents: They consist of the titrant (iodine dissolved in alcohol in an accurately defined concentration) and the optimally buffered solvent (an alcoholic solution containing sulfur dioxide and imidazole).
  Advantage: Greater titer stability and high titration rate.
  Disadvantage: Limited buffer capacity and limited sulfur dioxide content of the solvent.

With the **KFT Ipol** command, volumetric KF titrations are executed with voltametric endpoint indication.

Control during volumetric KF titration

During titration, reagent dosing is controlled in such a way that the predefined endpoint is reached as quickly and precisely as possible.

The reagent volume that has been dosed up to the endpoint determines reagent consumption, with which the water content of the sample can be calculated.

The volume steps and the rate of the reagent dosing are controlled using the difference between the current measured value and the predefined endpoint. This means that titration is slower and that smaller volumes are added in the control range.

The reagent is added in 3 phases during the titration:

- **Initial dosing** (**A**)
  As long as the **Control range** is not reached, the dosing rate is continually increased until the **Maximum dosing rate** is reached.
- **Continuous dosing** (**B**)
  During this phase, dosing is carried out continuously with the **Maximum dosing rate** until the **Control range** is reached.
- **Control range** (**C**)
  The closer the measured value is to the endpoint (**EP**), the slower the dosing in the **Control range**. Shortly before the endpoint (**EP**) is reached, dosing is carried out only with the **Minimum volume increment** parameter.

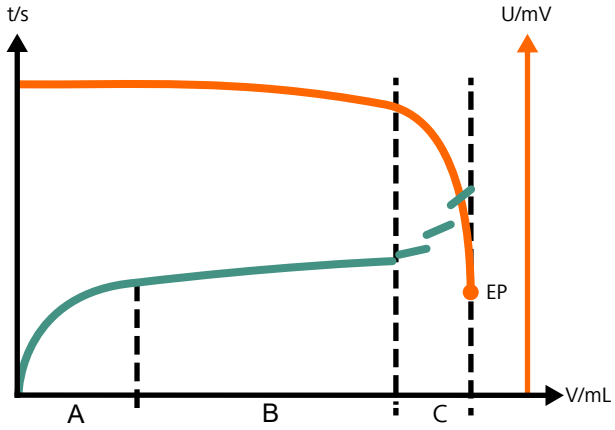


Figure 8 Control curve during a volumetric KF titration

A	**Initial dosing**	**B**	**Continuous dosing**
C	**Control range**	**EP**	**Endpoint**

Principle of the coulometric KF titration

With the coulometric Karl Fischer titration, the necessary iodine is directly and electrochemically generated in the electrolyte containing iodine ("electronic buret"). The voltage releases the respective stoichiometric quantity of iodine from the iodide-containing KF reagent through electrolysis.

No titer needs to be determined as the coulometric Karl Fischer titration is an absolute method. It must only be ensured that

- the reaction generating the iodine runs with a 100% current efficiency,
- no side reactions occur and
- oxidation or reduction lead to a defined oxidation level.

Iodine is generated with a generator electrode. There are 2 different types of generator electrodes:

- Generator electrode without diaphragm:
  The generator electrode without diaphragm is easy to handle and clean. Only one reagent is necessary. Since no moisture depots can set in the diaphragm, the coulometric titration cell is always quickly ready to use. The generator electrode without diaphragm does not have a cathode chamber.
- Generator electrode with diaphragm:
  The generator electrode with diaphragm should be used if the samples contain ketones and aldehydes. A generator electrode with diaphragm should also be used for reagents with a low conductivity (e.g. when chloroform is added) and for measurements in the lower trace range. The reagents consist of an anolyte and a catholyte that is added to the titration vessel or the cathode chamber.

With the **KFC** command, coulometric KF titrations are executed with voltametric endpoint indication.

Control during coulometric KF titration

During titration, the rate for the generation of iodine (generator rate) is controlled in such a way that the predefined endpoint is reached as quickly and precisely as possible.

The product of measured amount of current at the endpoint and titration duration (mA * s) is directly proportional to the generated iodine amount or titrated water quantity respectively.

The generator rate is controlled using the difference between the current measured value and the predefined endpoint. This means that a smaller amount of iodine is produced in the control range (influenced by the **Minimum generator rate**).

Outside the control range, the generator rate is continuously increased until the **Maximum generator rate** is reached.

The rate for the generation of iodine is controlled in 3 phases during titration:

- **Initial rate** (**A**)
  As long as the **Control range** is not reached, the generator rate is continually increased until the **Maximum generator rate** is reached.
- **Continuous rate** (**B**)
  During this phase, iodine is generated continuously with the **Maximum generator rate** until the **Control range** is reached.
- **Control range** (**C**)
  The closer the measured value is to the endpoint **EP**, the lower the quantities of iodine are that are generated in the **Control range**. Shortly before the endpoint **EP** is reached, iodine is generated only at the **Minimum generator rate**.

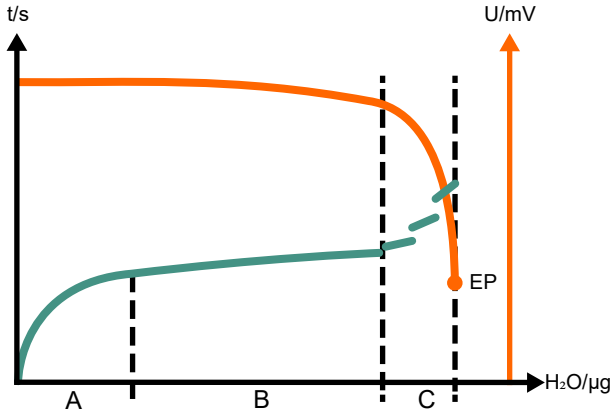
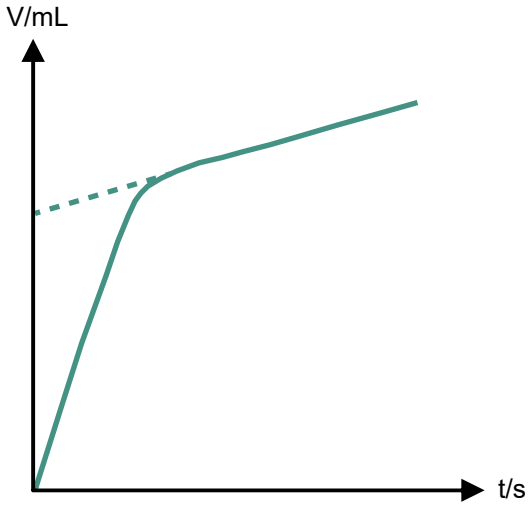


Figure 9 Control curve during a coulometric KF titration

A	**Initial dosing**	**B**	**Continuous dosing**
C	**Control range**	**EP**	**Endpoint**

Post-drift correction

The **EVAL LINEAR REGRESSION** command can be used for post-drift correction with Karl Fischer titrations. A linear regression is carried out in the same subsample over a defined measuring point range in the measuring point list. If the quantity **Time** is selected for the parameter **Quantity on the x-axis** and the quantity **Water** (KFC) or **Volume** (KFT Ipol) is selected for the **Quantity on the y-axis** parameter, then the water content of the sample can be determined with the command variable '**Intercept.Result**.*command name*.



Additional information on the **EVAL LINEAR REGRESSION** command: *(see "EVAL LINEAR REGRESSION – Parameters", chapter 5.11.8.68, page 776)*

See also

KFC – Command variables (chapter 5.11.8.11.2, page 596)

KFC – Properties (chapter 5.11.8.11, page 586)

KFT – Command variables (chapter 5.11.8.10.3, page 582)

KFT – Properties (chapter 5.11.8.10.1, page 568)

Karl Fischer titration coulometric – Run (chapter 5.11.8.11.1, page 594)

Karl Fischer titration volumetric – Run (chapter 5.11.8.10.2, page 580)

5.11.8.10 Conditioning – Principle

The closed titration cell in which the water content determination is carried out should initially be as free of water as possible in order to have a defined and constant starting point.

This is achieved by conditioning the reagent in the titration cell by adding iodine.

For titration methods with conditioning, the following commands must be processed prior to the titration command (**KFC**, **KFT Ipol**, **SET Ipol**), which must contain the **Parameters for conditioning**:

- **COND ON** *(see "COND ON – Parameters", chapter 5.11.8.13, page 604)*: Start conditioning.
- **COND CHECK** *(see "COND CHECK – Parameters", chapter 5.11.8.15, page 606)*: Monitor conditioning that was started with the **COND ON** command.

The criteria for determining when the titration cell is conditioned (i.e. when it is ready for water content determination) are defined in the titration command in the (**Start drift**, **Stabilizing time**) under **Parameters for conditioning**.

The transition from conditioning to titration is defined in the **COND CHECK** command under **Titration start** *(see "COND CHECK – Parameters", chapter 5.11.8.15, page 606)*. If the titration is to be started automatically when a sample addition is recognized, the **Recognition of sample addition** check box must also be activated under **Parameters for conditioning** for the **KFC** command or the **KFT Ipol** command.

After conditioning, the titration is carried out as defined in the titration command parameters.

Conditioning after the last subsample

If the titration cell is to be conditioned further after completing the titration, another **COND ON** command must be inserted in the process run after the **KFC** command, the **KFT Ipol** command or the **SET Ipol** command. This means that the titration cell is further conditioned even without a running subsample.

The next subsample can be started when the reconditioning is ongoing. A running work system can be recognized by the icon on the left

side of the program window. The work system that is reconditioning can be accessed directly by clicking on . The conditioning status and the measured values are displayed on the work system and the reconditioning can be stopped.

Current status

If the selected work system is being used for conditioning, the current measured values for the ongoing conditioning process are displayed in **Current status**.

The conditioning status of the ongoing process (e.g. **Conditioning OK** or **Conditioning not OK**) and the stability of the drift are also shown in the window. In this way, it can be recognized immediately whether conditioning conditions have been met.

Further information on the icons that are displayed with the measured values: *(see "Displaying live data and controlling the run", chapter 5.10.10, page 316)*

See also

KFT – Command variables (chapter 5.11.8.10.3, page 582)

KFT – Properties (chapter 5.11.8.10.1, page 568)

SET – Command variables (chapter 5.11.8.6.3, page 530)

SET – Properties (chapter 5.11.8.6.1, page 512)

5.11.8.10.1 KFT – Properties

The **KFT Ipol** command is used to execute volumetric **K**arl **F**ischer **t**itration (KFT). The water content determination according to Karl Fischer is carried out by an endpoint titration with voltametric measurement.

The determination can be paused manually during the execution of a **KFT Ipol** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

After selecting the **KFT Ipol** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **KFT Ipol** command:

Parameters

The **Parameters for conditioning** are only effective if the Karl Fischer titration is carried out with conditioning. The **COND ON** and **COND CHECK** commands must be present in the process sequence before the **KFT Ipol** command for this purpose.

Parameters for conditioning	
Start drift	The **Start drift** is a threshold value that the volume drift needs to be below during the entire **Stabilizing time** so that the **Conditioning OK** status is reached. The value should be adjusted to the titrant and humidity conditions.
Stabilizing time	The **Stabilizing time** starts as soon as the volume drift falls below the **Start drift**. If the volume drift has fallen below the **Start drift** during the entire **Stabilizing time**, then the status **Conditioning OK** is reached after the **Stabilizing time** has elapsed. As soon as the volume drift once again exceeds the **Start drift** during the **Stabilizing time**, the **Stabilizing time** is re-initialized. Metrohm recommends setting a value of at least 3 s when using **Recognition of sample addition**. If an extraction method with oven is used for the water content determination, Metrohm recommends increasing the value to at least 10 s.

Parameters for conditioning	
Recognition of sample addition (only OMNIS instruments)	The start of the titration with **Recognition of sample addition** is suitable for samples that can be added quickly in the titration cell. If this option is activated and a sample addition is recognized, then titration starts automatically in the status **Conditioning OK** (without waiting for the **Sample addition time**). In order to obtain correct results when working with the **Recognition of sample addition**, the following preconditions must be met: ▪ The electrode and the buret tip must be positioned correctly, as described in the OMNIS Titrator product manual (8.1001.8002) under *Mounting the volumetric Karl Fischer titration cell*. ▪ The sample in the measuring cell must be well-mixed. In order to do so, the stirring rate of the stirrer must be adjusted. ▪ If the **Recognition of sample addition** function is enabled, then the **Correction with volume drift** must not be set to **Automatic**. **Note:** The **Recognition of sample addition** function exists only in OMNIS instruments.
Threshold value	The volume drift must have exceeded the **Threshold value** within a short time in order for the conditioning to stop automatically and for the process sequence to continue out of the **Conditioning OK** status due to the **Recognition of sample addition**.
Sample addition time	The **Sample addition time** is a waiting time between the end of the conditioning and the start of the titration which is waited for before the sample addition into the titration cell. If the titration was started with **Recognition of sample addition**, then the **Sample addition time** is skipped.
Correction with volume drift	The correction volume is subtracted from the endpoint volume with the **Correction with volume drift** parameter. The use of the **Correction with volume drift** is displayed in the raw data. The following options can be selected: ▪ **Off**: No correction of the endpoint volume is taking place. ▪ **Automatic**: The correction volume is calculated with the volume drift that was determined during conditioning. This option must **not** be used in combination with the **Recognition of sample addition**. ▪ **Manual**: The correction volume is calculated with the following **Volume drift** parameter. The influx of humidity can cause a volume drift of up to 20 µL/min even with leakproof titration cells.

Parameters for conditioning	
Volume drift	The **Volume drift** parameter is only active if the **Correction with volume drift** was activated with **Manual**. Metrohm recommends determining the value of the volume drift in advance with a blind titration over several minutes with the equipment used.
Conditioning stop volume	If the **Conditioning stop volume** is reached during conditioning, the determination is canceled with a message as it has to be assumed that there is a problem. The conditioning stop volume must be adjusted to the volume of the titration vessel in order to prevent any overflow.
Conditioning stop time	If the **Conditioning stop time** is reached during conditioning, the determination is canceled with a message as it has to be assumed that there is a problem.

Start conditions	
Signal drift initial measured value	The initial measured value is applied as soon as the signal drift falls below the defined value or no later than after the maximum waiting time has expired. **Off** deactivates the drift control.
Minimum waiting time	If drift control is enabled, the initial measured value will not be applied until after the minimum waiting time has expired at the earliest, and the measurement will be aborted, even if it has already fallen below the **Signal drift initial measured value**.
Maximum waiting time	**Drift control enabled:** If the signal drift does not fall below a defined value before the maximum waiting time has expired, then the initial measured value is applied after the maximum waiting time has expired, and the measurement is aborted. **Drift control disabled:** The initial measured value is applied after the maximum waiting time has expired and the measurement is aborted.
Start volume	The solution is added before the start of titration until the start volume is reached. The following stop conditions are checked while dosing the start volume: ▪ **Stop volume** ▪ **Stop time**

Start conditions	
Dosing rate start volume	Rate at which dosing takes place until the start volume has been reached. If a **Maximum dosing rate** is defined for dosing port 1 of the cylinder unit that is smaller than the **Dosing rate start volume** in the **Equipment** work area, then the maximum dosing rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the cylinder unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Pause	Waiting time, e.g. for the measured value to stabilize after start or as reaction time after dosing a start volume. The pause follows at the end of all the start conditions.

Endpoint control parameters	
Endpoint at	Measured value for the endpoint. The default value 250 mV with a polarization current **I(pol) DC** of 50 µA is valid for most applications.
Titration rate	The titration rate can either be determined using 4 predefined parameter sets, or the values for the titration parameters can be defined individually. ▪ **Slow**: Parameter set for titrations for which the finest details are to be visible. This can, however, lead to an increase in noise, which may result in unwanted equivalence points. ▪ **Optimal 1-component reagents**: Parameter set that has been optimized for the most common applications with 1-component reagents. ▪ **Optimal 2-component reagents**: Parameter set that has been optimized for the most common applications with 2-component reagents. ▪ **Fast**: Parameter set for not very critical, fast titrations. ▪ **Enter values**: The values for the titration parameters must be defined individually. If a predefined parameter set is selected for the titration rate, the following parameters are displayed but they cannot be edited: ▪ **Control range** ▪ **Maximum dosing rate** ▪ **Minimum volume increment** The values used can be read in the corresponding parameters. **Note**: If reagents with low levels of methanol are used, Metrohm recommends using the **Optimal 2-component reagents** rate and enter a value of 20 µA in the **I(pol) DC** parameter.

Endpoint control parameters	
Control range	The volume steps and the rate of the reagent dosing are controlled using the difference between the current measured value and the predefined endpoint. This means that titration is slower and that smaller volumes are added (affected by the **Minimum volume increment**) in the control range. Outside the control range, the dosing rate is continuously increased until the **Maximum dosing rate** is reached. With **Unlimited**, the entire measuring range is considered as **Control range**. **Note**: The setting **Unlimited** is identical to the setting **Off** in previous Metrohm applications. This parameter influences the accuracy with which the endpoint is reached. The larger the control range, the longer the titration will take but the more accurately the endpoint is approached. The control range can be reduced if accuracy has a subordinated role and titration should be carried out faster.
Maximum dosing rate	Maximum rate of acceleration outside the control range. Depending on the measured value change, it may not be possible to reach the maximum dosing rate. If a smaller **Maximum dosing rate** is defined for the dosing port of the cylinder unit in the **Equipment** work area, then that rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the cylinder unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are dosed or if tubing is used that is thinner than standard tubing, then the dosing rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Minimum volume increment	Minimum volume increment that is used for dosing at the beginning of the titration and in the control range at the end of the titration. The smaller the selected increment, the slower the titration and the higher the accuracy.

Endpoint control parameters	
Stop criterion	Once the specified endpoint has been reached, the procedure pauses after the final dosing while awaiting the selected stop criterion to be reached. After this, the endpoint is considered to have been reached and the titration is stopped. The following stop criteria can be selected: ▪ **Stop drift**: Once the specified endpoint has been reached and the volume drift falls below the defined **Stop drift**, the endpoint is applied and the titration is finished. ▪ **Relative stop drift**: Once the specified endpoint has been reached and the volume drift falls below the value of the sum of the **Relative stop drift** and volume drift at the start of the titration, the endpoint is applied and the titration is finished. ▪ **Delay time**: Once the specified endpoint has been reached and the selected **Delay time** has passed, the endpoint is applied and the titration is finished. ▪ **Off**: The titration is canceled only by the stop conditions. No endpoint data is saved as raw data.

Titration parameters	
Titration direction	Selection of the titration direction: ▪ **Positive**: In the direction of positive measured value change ▪ **Negative**: In the direction of negative measured value change ▪ **Automatic**: The titration direction is calculated with the initial measured value and the set endpoint. Metrohm recommends specifying the titration direction. If the titration direction is specified, a message is shown if the actual titration direction does not correspond to the one specified. For Karl Fischer titration with a positive polarization current of the electrode (**I(pol) DC**), the titration direction is **Negative**.
Extraction time	During the **Extraction time**, no endpoint is applied and the titration is not ended, even if the endpoint and the stop criterion have already been reached. The extraction time starts from the moment all start conditions have been processed. It is advisable to enter an **Extraction time**, e.g. for the titration of sparingly soluble samples or when performing an external extraction with oven.

Titration parameters	
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The manually entered temperature is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the titration, even if the time interval has not yet been reached.
I(pol) DC	The polarization current **I(pol) DC** (Direct Current) is the current that is applied to the polarizable electrode during voltametric measurement. **Note**: For OMNIS instruments, Metrohm recommends entering the current in increments of 0.5 µA. For Metrohm USB instruments an increment of 0.5 µA **must** be observed. The **Endpoint at** and the **Control range** may also need to be adjusted when the polarization current is changed.
Carry out electrode check	The electrode check is carried out for polarizable electrodes during the transition from an inactive normal status to conditioning or titration. It checks within a few seconds whether an electrode is connected and whether no short circuit is present. If the titration is carried out with conditioning, then the check is carried out only at the start of conditioning.
Filling rate	Rate at which the cylinder is filled. If a smaller **Maximum filling rate** is defined for the fill port of the cylinder unit in the **Equipment** work area, then that rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the cylinder unit used. If this should be the case, then the instrument will reduce the rate. If air bubbles form during the aspiration of the solution, then the filling rate needs to be reduced accordingly so that the dosing drive it is not overloaded.

Stop conditions	
Stop volume	The titration is canceled as soon as the defined volume has been dosed since the start of the titration (including start conditions). The volume must be adjusted to the size of the titration vessel to prevent it from overflowing. In addition, the **Stop volume** should always be smaller than the cylinder volume to avoid refilling during the titration. **Off** disables this stop condition.
Stop time	The titration is canceled as soon as the defined time has elapsed since the start of the determination (including start conditions). **Off** disables this stop condition.

Fixed point evaluation	
Define fixed points	The subsection for defining the fixed points is opened. *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*
Specified quantity	Selection of the specified quantity for the calculation of the fixed point from the measuring point list: ▪ **Potential** The values **Time**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Volume** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Volume** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified volume.
Fixed point at	Specified measured value for the calculation of the fixed point.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Volume** ▪ **Potential** ▪ **Drift** ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Volume** (default value) ▪ **Potential** ▪ **Drift** ▪ **Temperature**

Chart – y2-axis	
Display y2-axis	If this option is activated, the second y-axis is shown for displaying another quantity as a curve.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Volume** ▪ **Potential** (default value) ▪ **Drift** ▪ **Temperature**

Curve simulation	
Curve selection	Simulated curves can be used with OMNIS instruments to check the determination run. The titration sequence is defined by the set parameters. The simulation must be deactivated before analyzing real samples. The following simulation curves can be selected: ▪ **None** (default value) No simulation curve (the curve simulation is deactivated). ▪ **KFT with conditioning** Titration curve for KF methods with conditioning, i.e. with the commands **COND ON** and **COND CHECK**. The endpoint is reached at approx. 10% of the buret volume. ▪ **KF titration** Titration curve for KF titration without conditioning. The endpoint is reached at approx. 50% of the buret volume.

Before analyzing real samples, deactivate the curve simulation. No curve simulation is available for instruments of the **Titrando** type.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift initial measured value**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Dosing rate start volume**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min
- **Endpoint at**
  Minimum value: –1,200.0 mV
  Maximum value: 1,200.0 mV

- **Maximum dosing rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s
- **I(pol) DC**
  Minimum value: –122.5 µA
  Maximum value: 122.5 µA
  Permitted increment: 0.5 µA
- **Filling rate**
  Minimum value: 0.01 mL/min
  Maximum value: 166.00 mL/min

Execute with

In order for a **KFT** command to be executed, the corresponding functional units need to be assigned to the command.

- Dosing unit to which the solution required for titration is connected: **Dosing Drive** with connected **Cylinder Unit**, **800 Dosino** with connected **807 Dosing Unit**, **805 Dosimat** with connected **806 Exchange Unit** or **Internal Dosing Drive** with connected **806 Exchange Unit**
- Digital or analog measuring input to which the sensor required for titration is connected:
  Measuring Module Digital, **Measuring Module Analog**, **Measuring Interface Analog** or **Interface Coulometry**

After a functional unit for the command has been selected, the following additional parameters appear:

For **Dosing Drive**:	
Dosing port	Port that is to be used to dose a volume increment. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1 (default value). ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2.

For **Measuring Module Analog**:	
Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Measuring Interface Analog**:	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: **Pol./Temp.**: Measurement with a polarizable electrode and/or a temperature sensor. **Pol.**: Measurement with a polarizable electrode.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Interface Coulometry**:	
Measuring input	Selection of the analog measuring input. **Ind./Temp.**: Measurement with an analog electrode and/or a temperature sensor.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

COND CHECK – Parameters (chapter 5.11.8.15, page 606)

COND OFF – Parameters (chapter 5.11.8.14, page 605)

COND ON – Parameters (chapter 5.11.8.13, page 604)

Commands – Definition (chapter 5.11.8, page 429)

Conditioning – Principle (chapter 5.11.8.10, page 567)

Creating and editing a method (chapter 5.11.3.3, page 418)

KFT – Command variables (chapter 5.11.8.10.3, page 582)

Karl Fischer titration volumetric – Run (chapter 5.11.8.10.2, page 580)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

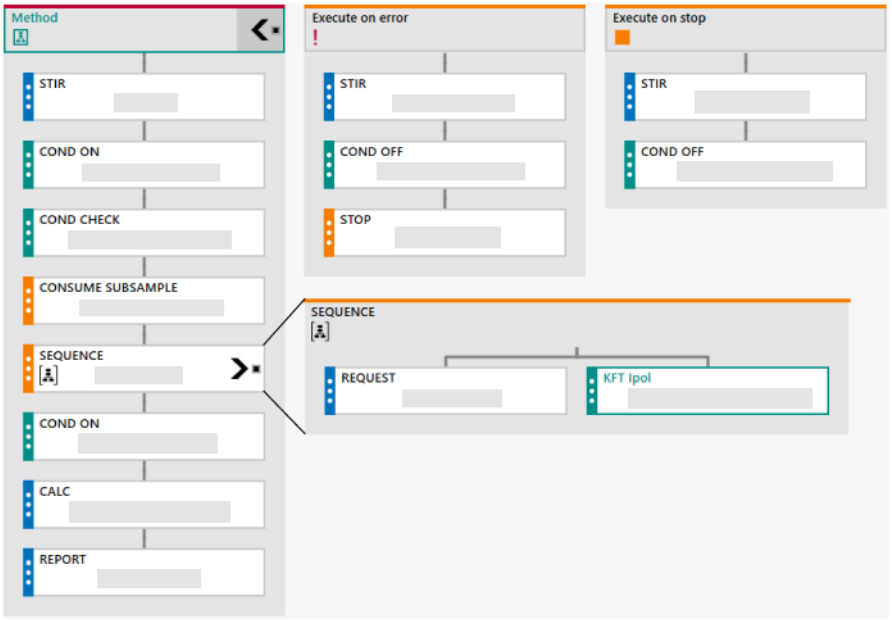
5.11.8.10.2 Karl Fischer titration volumetric – Run

The **KFT Ipol** command can be executed with and without conditioning.

If conditioning is necessary, the conditioning commands **COND ON** (Start conditioning) and **COND CHECK** (Monitor conditioning) must be inserted before the **KFT Ipol** command.

If reconditioning is necessary, a **COND ON** command must be inserted in the method again after the **KFT Ipol** command.

A standard method for **KFT Ipol** with conditioning may look as follows:



The **KFT Ipol** command is executed in the following steps:

1 – Preconditioning

A KFT work system can be conditioned by inserting a **COND ON** command and a **COND CHECK** command before the **KFT Ipol** command in the KF method.

The transition from conditioning to titration is defined in the **COND CHECK** command under **Titration start**. If **Manual / After sample addition** was selected, the titration can be started manually after conditioning with the **[Start titration]** button in the live data of the determination. Or the titration is automatically started at the recognition of a sample addition if the check box **Recognition of sample addition** is activated in the referenced titration command. If **Automatic after COND OK** was selected, the titration starts automatically as soon as the conditioning conditions **Start drift** and **Stabilizing time** of the referenced titration command are fulfilled and the **Sample addition time** has elapsed.

2 – Determining the initial measured value

The initial measured value (measured value before start of pre-dosing) is determined according to the parameters under **Start conditions**, either drift-controlled or after a maximum waiting time has elapsed.

This step should be carried out e.g. to determine the titration direction.

3 – Dosing the start volume

If a **Start volume** was defined in **Start conditions**, it is pre-dosed before the actual titration. The defined **Pause** time is then observed.

4 – Carrying out the titration with the set control parameters and titration parameters

The titration is carried out according to the parameters defined under **Endpoint control parameters** and **Titration parameters**.

- **Fixed point evaluation**
  Optionally, up to 9 fixed points can be defined in **Fixed point evaluation** that are calculated from the measuring point list during the titration.
- **Graph – … axes**
  Optionally, different quantities can be selected for the x-axis and y-axis. In addition, a y2-axis can be displayed.

5 – Completing the titration

The titration is completed as usual as soon as the endpoint defined in **Endpoint control parameters** and the defined stop criterion are reached.

The conditions defined under **Stop conditions** are constantly monitored during the titration. By defining one or more stop conditions, the user makes sure that e.g. the titration vessel does not overflow if the endpoint is not reached or if the stop criterion is never met. The titration is canceled if one of these conditions applies.

A running titration can be canceled by a manual cancellation or with the emergency stop or in case of an error.

6 – Reconditioning

A KFT work system can be conditioned further after the determination has ended (reconditioning) by inserting another **COND ON** command in the KF method at the end of a process sequence after a **KFT Ipol** command.

In doing so, the titration cell is conditioned even without a running sub-sample. Conditioning can be stopped manually in the window of the respective work system.

See also

COND CHECK – Command variables (chapter 5.11.8.15.1, page 608)

COND CHECK – Parameters (chapter 5.11.8.15, page 606)

COND OFF – Parameters (chapter 5.11.8.14, page 605)

COND ON – Parameters (chapter 5.11.8.13, page 604)

Conditioning – Principle (chapter 5.11.8.10, page 567)

KFT – Command variables (chapter 5.11.8.10.3, page 582)

KFT – Properties (chapter 5.11.8.10.1, page 568)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

5.11.8.10.3 KFT – Command variables

The following variables are generated by the **KFT Ipol** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Driftvalue.DriftCorrection**.*Command name*' Volume drift that was used for correcting the EP volume. When working with conditioning, this volume drift is used for calculating the EP volume correction if the **Correction with volume drift** parameter was activated (**Automatic** or **Manual**). Unit: µL/min
'**Driftvalue.EP{1}**.*Command name*' Volume drift of the endpoint. Unit: µL/min
'**Driftvalue.Final**.*Command name*' Volume drift for the last measuring point in the measuring point list. Unit: µL/min

Command variables
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**Duration.DriftCorrection**.*Command name*' Period from the end of conditioning until the end of the titration. When working with conditioning, this time period is used for calculating the EP volume correction if the **Correction with volume drift** parameter was activated (**Automatic** or **Manual**). Unit: s
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Index.EP{1}**.*Command name*' Index of the endpoint. Unit: None
'**Index.FP{x}**.*Command name*' (x = 1–9) Index of the fixed point. Unit: None
'**Measvalue.EP{1}**.*Command name*' Measured value of the endpoint. Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable
'**Measvalue.FP{x}**.*Command name*' (x = 1–9) Measured value of the fixed point. Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable

Command variables
'**Temperature.EP{1}**.*Command name*' Temperature associated with the endpoint. Unit: °C
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Temperature.FP{x}**.*Command name*' (x = 1–9) Temperature associated with the fixed point. Unit: °C
'**Time.EP{1}**.*Command name*' Time stamp associated with the endpoint. Unit: s
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Time.FP{x}**.*Command name*' (x = 1–9) Time stamp associated with the fixed point. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of the measured value.
'**Volume.DriftCorrection**.*Command name*' Volume that was calculated for the drift-based correction of the EP volume. The correction volume is calculated by multiplying the volume drift with the period from the end of conditioning until the end of the titration. When working with conditioning, this volume is used for the EP volume correction if the **Correction with volume drift** parameter was activated (**Automatic** or **Manual**). Unit: mL
'**Volume.EP{1}**.*Command name*' The volume that is dosed until the endpoint is reached. When working with conditioning, this value is corrected by the **Volume.DriftCorrection**.'*Command name*' volume if the parameter **Correction with volume drift** was activated (**Automatic** or **Manual**). Unit: mL

Command variables
'**Volume.Final**.*Command name*' End volume after processing the command, i.e. total dosed volume at the end of the command. Unit: mL
'**Volume.FP{x}**.*Command name*' (x = 1–9) The volume that is dosed until the fixed point is reached. Unit: mL

In the case of variables with index **{x}**, the index **{1}** is set automatically at the time of insertion in a formula.

Equipment variables
'**Concentration.CurrentSolution**.*Command name*' Concentration of the solution used that is dosed with the dosing unit or buret (corresponds to the concentration of component 1 in the solution used). Unit: Defined in the '**Unit.Concentration.CurrentSolution**.*Command name*' variable
'**Diameter.AspirationTube.CurrentSolution**.*Command name*' Diameter of the aspiration tubing in the bottle of the solution used. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing in the bottle of the solution used. Unit: cm
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.
'**Name.CurrentSolution**.*Command name*' Name of the solution used with the dosing unit. The name can only be defined by the user in the properties of the solution if a bottle cap multi-use is used.
'**Titer.CurrentSolution**.*Command name*' Titer of the solution used that is dosed with the dosing unit. For Karl Fischer titrants, the titer usually shows how much water (in mg) can be titrated in 1 mL of titrant. Unit: Defined in the '**Unit.Titer.CurrentSolution**.*Command name*' variable

Equipment variables
'**Unit.Concentration.CurrentSolution**.*Command name*' Unit of the concentration of the solution used that is dosed with the dosing unit (corresponds to the unit of the concentration of component 1 in the solution used). The unit of the concentration can only be defined by the user in the properties of the solution if a bottle cap multi-use is used.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer of the solution used.

See also

KFT – Properties (chapter 5.11.8.10.1, page 568)

Karl Fischer titration volumetric – Run (chapter 5.11.8.10.2, page 580)

5.11.8.11 KFC – Properties

The **KFC** command is a titration command for the **c**oulometric **K**arl **F**ischer titration (KFC). The coulometric water content determination is used mainly to determine small amounts of water.

With **KFC**, the necessary iodine is directly and electrochemically generated in the electrolytes containing iodide ("electronic buret"). Between the amount of electric charge and the amount of generated iodine, there is a strictly quantitative relationship, which is used for high-precision dosing of the iodine. The coulometric Karl Fischer titration is an absolute determination and is carried out by an endpoint titration with voltametric measurement.

The determination can be paused manually during the execution of a **KFC** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

After selecting the **KFC** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **KFC** command:

Parameters

The **Parameters for conditioning** are only effective if the Karl Fischer titration is carried out with conditioning. The commands **COND ON** and **COND CHECK** must be present in the process sequence before the **KFC** command for this purpose.

Parameters for conditioning	
Start drift	The **Start drift** is a threshold value below which the amount drift needs to remain during the entire **Stabilizing time** so that the **Conditioning OK** status can be achieved. The value should be adjusted to the titrant and humidity conditions.
Stabilizing time	The **Stabilizing time** starts as soon as the amount drift falls below the **Start drift**. If the amount drift has fallen below the **Start drift** during the entire **Stabilizing time**, then the status **Conditioning OK** is reached after the **Stabilizing time** has elapsed. The **Stabilizing time** is restarted as soon as the amount drift once again exceeds the **Start drift** during the **Stabilizing time**. Metrohm recommends setting a value of at least 2 s when using **Recognition of sample addition**. If an extraction method with oven is used for the water content determination, Metrohm recommends increasing the value to at least 60 s.
Recognition of sample addition	The start of the titration with **Recognition of sample addition** is suitable for samples that can be added quickly in the titration cell. If this option is activated and a sample addition is recognized, then titration starts automatically in the status **Conditioning OK** (without waiting for the **Sample addition time**). In order get correct results when working with the **Recognition of sample addition**, the following prerequisites must be met: ▪ The electrodes must be positioned correctly, as described in **Equipping the coulometer cell** in the product manual of the 851 Titrando (8.851.8004) and in *Equipping the coulometric Karl Fischer titration cell* in the product manual of the OMNIS Coulometer (8.1020.8002). ▪ The sample in the measuring cell must be well-mixed. In order to do so, the stirring rate of the stirrer must be adjusted.
Threshold value	The **Potential** must have exceeded the **Threshold value** within a short time in order for the conditioning to stop automatically and for the process sequence to continue out of the **Conditioning OK** status due to the **Recognition of sample addition**.
Sample addition time	The **Sample addition time** is a waiting time between the end of the conditioning and the start of the titration which is waited for before adding the sample into the titration cell. If the titration was started with **Recognition of sample addition**, then the **Sample addition time** is skipped.

Parameters for conditioning	
Correction with amount drift	With the **Correction with amount drift** parameter, the correction water quantity is subtracted from the endpoint water quantity. The use of the **Correction with amount drift** is displayed in the raw data. The following options can be selected: ▪ **Off**: No correction of the endpoint water quantity is taking place. ▪ **Automatic**: The correction water quantity is calculated with the amount drift that was determined during conditioning. ▪ **Manual**: The correction water quantity is calculated with the following **Amount drift** parameter. The influx of humidity can cause an amount drift of up to 20 µg/min, even with leak-tight titration cells.
Amount drift	The **Amount drift** parameter is only active if the **Correction with amount drift** was activated with **Manual**. Metrohm recommends determining the value of the amount drift in advance with a blind titration over several minutes with the equipment used.
Conditioning stop time	If the **Conditioning stop time** is reached during conditioning, the determination is canceled with a message as it has to be assumed that there is a problem.
Start conditions	
Pause	Waiting time before the start of the recording of the titration curve.
Endpoint control parameters	
Endpoint at	Measured value for the endpoint. The default value 50 mV with a polarization current **I(pol) AC** of 10 µA is valid for most applications.

Endpoint control parameters	
Titration rate	The titration rate can either be determined using 3 predefined parameter sets, or the values for the titration parameters can be defined individually. ▪ **Slow**: Parameter set for titrations for which the finest details are to be visible. This can, however, lead to an increase in noise, which may result in unwanted equivalence points. ▪ **Optimal**: Parameter set that has been optimized for the most common applications. ▪ **Fast**: Parameter set for not very critical, fast titrations. ▪ **Enter values**: The values for the titration parameters must be defined individually. If a predefined parameter set is selected for the titration rate, the following parameters are displayed but they cannot be edited: ▪ **Control range** ▪ **Maximum generator rate** ▪ **Minimum generator rate** The values used can be read in the corresponding parameters.
Control range	The generator rate is controlled using the difference between the current measured value and the predefined endpoint. This means that a smaller amount of iodine is produced in the control range (influenced by the **Minimum generator rate**). Outside the control range, the generator rate is continuously increased until the **Maximum generator rate** is reached. With **Unlimited**, the entire measuring range is considered as the control range. This parameter influences the accuracy with which the endpoint is reached. The larger the control range, the longer the titration will take but the more accurately the endpoint is approached.
Maximum generator rate	Maximum rate at which iodine is generated outside the control range.
Minimum generator rate	Minimum rate at which iodine is generated within the control range. The smaller this rate, the slower the titration and the higher the accuracy.

Endpoint control parameters	
Stop criterion	Once the specified endpoint and the selected stop criterion has been reached, the endpoint is applied and the titration is finished. The following stop criteria can be selected: ▪ **Stop drift**: Once the specified endpoint has been reached and the amount drift falls below the selected **Stop drift**, the endpoint is applied and the titration is finished. ▪ **Relative stop drift**: Once the specified endpoint has been reached and the amount drift falls below the value of the sum of the **Relative stop drift** and amount drift at the start of the titration, the endpoint is applied and the titration is finished. ▪ **Delay time**: Once the specified endpoint has been reached and the selected **Delay time** has passed, the endpoint is applied and the titration is finished. ▪ **Off**: The titration is canceled only by the stop condition **Stop time**. No endpoint data is saved as raw data.
Titration parameters	
Extraction time	During the **Extraction time**, no endpoint is applied and the titration is not ended, even if the endpoint and the stop criterion have already been reached. The extraction time starts from the moment all start conditions have been processed. It is advisable to enter an **Extraction time**, e.g. for the titration of sparingly soluble samples or when performing an external extraction with oven.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The manually entered temperature is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the **Automatic** or **Manual** setting has been selected.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the titration, even if the time interval has not yet been reached.

Titration parameters	
I(pol) AC	The polarization current **I(pol) AC** (Alternating Current) is the current that is applied to the indicator electrode during voltametric measurement. The **Endpoint at** and the **Control range** may need to be adjusted when the polarization current (5, 10, 20, 30 µA) is changed.
Carry out electrode check	▪ **Indicator electrode** (polarizable metal electrode): For titration without conditioning, the check is carried out before the start of the titration, during the transition from the inactive normal status to the titration. For a titration with conditioning, the check is carried out before the start of conditioning. It checks within a few seconds whether an electrode is connected and whether a short circuit is present. ▪ **Generator electrode**: In cases of titrations without conditioning, the check is carried out during the determination. For a titration with conditioning, the check is carried out during conditioning and during the determination. It checks whether an electrode is connected and whether the resistance in the electrode is too high.
Generator type	Selection of the generator type. The following generator electrode types can be selected: **Without diaphragm**: for standard applications with correspondingly suitable reagents. **With diaphragm**: for applications with reagents which require the generator electrode with diaphragm, e.g. reagents for water content determinations in ketones.
Generator current	Polarization current that is applied at the generator electrode to generate iodine. If **Automatic** is selected, the current is automatically adapted to the conductivity of the reagent and reduced near the endpoint in a controlled manner. **Without diaphragm**: Metrohm recommends to keep the default value of **400 mA** for the generator current and not to enable **Automatic**. **With diaphragm**: Metrohm recommends to keep the default value **Automatic** for the **Generator current**.
Stop conditions	
Stop time	The titration is canceled as soon as the defined time has elapsed since the start of the determination (including start conditions). **Off** disables this stop condition.

Fixed point evaluation	
Define fixed points	The subsection for defining the fixed points is opened. *(see "Curves – Fixed point evaluation", chapter 5.10.11.3, page 327)*
Specified quantity	Selection of the specified quantity for the calculation of the fixed point from the measuring point list: ▪ **Potential** The values **Time**, **Water** and **Temperature** are interpolated from the measuring point list for the specified potential. ▪ **Time** The values **Potential**, **Water** and **Temperature** are interpolated from the measuring point list for the specified time. ▪ **Water** The values **Potential**, **Time** and **Temperature** are interpolated from the measuring point list for the specified water content.
Fixed point at	Specified measured value for the calculation of the fixed point.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Water** ▪ **Potential** ▪ **Drift** ▪ **Temperature** ▪ **Charge** ▪ **Ugen** ▪ **Igen**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Water** (default value) ▪ **Potential** ▪ **Drift** ▪ **Temperature** ▪ **Charge** ▪ **Ugen** ▪ **Igen**

Chart – y2-axis	
Display y2-axis	If this option is activated, the 2nd y-axis is shown for displaying another quantity as a curve.

Chart – y2-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the 2nd y-axis: ▪ **Time** ▪ **Water** ▪ **Potential** ▪ **Drift** (default value) ▪ **Temperature** ▪ **Charge** ▪ **Ugen** ▪ **Igen**

Curve simulation	
Curve selection	Simulated curves can be used with OMNIS instruments to check the determination run. The titration sequence is defined by the set parameters. The simulation must be deactivated before analyzing real samples. The following simulation curves can be selected: ▪ **None** (default value) No simulation curve (the curve simulation is deactivated). ▪ **KFC titration** Titration curve for KFC titration.

Additional information on the parameters (e.g., input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **KFC** command to be executed, the corresponding functional unit must be assigned to it:

Measuring Module Coulometry or **Interface Coulometry**

The following parameters must also be defined:

For **Measuring Module Coulometry**:	
Sensor name	Selection of the indicator electrode of the **Polarizable metal electrode** type to be used at the **INPUT 1** measuring input for the titration. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the sensor of the **Temperature sensor** type that is to measure the temperature at the measuring input **INPUT 2** during the analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Interface Coulometry**:	
Measuring input	Selection of the analog measuring input. **Ind./Temp.**: Measurement with an analog electrode and/or a temperature sensor.
Sensor name	Selection of the indicator electrode of the **Polarizable metal electrode** type to be used for the titration. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the sensor of the **Temperature sensor** type that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

BRC CC Ipol – Properties (chapter 5.11.8.2.1, page 435)

COND CHECK – Command variables (chapter 5.11.8.15.1, page 608)

COND CHECK – Parameters (chapter 5.11.8.15, page 606)

COND OFF – Parameters (chapter 5.11.8.14, page 605)

COND ON – Parameters (chapter 5.11.8.13, page 604)

Commands – Definition (chapter 5.11.8, page 429)

Conditioning – Principle (chapter 5.11.8.10, page 567)

Creating and editing a method (chapter 5.11.3.3, page 418)

KFC – Command variables (chapter 5.11.8.11.2, page 596)

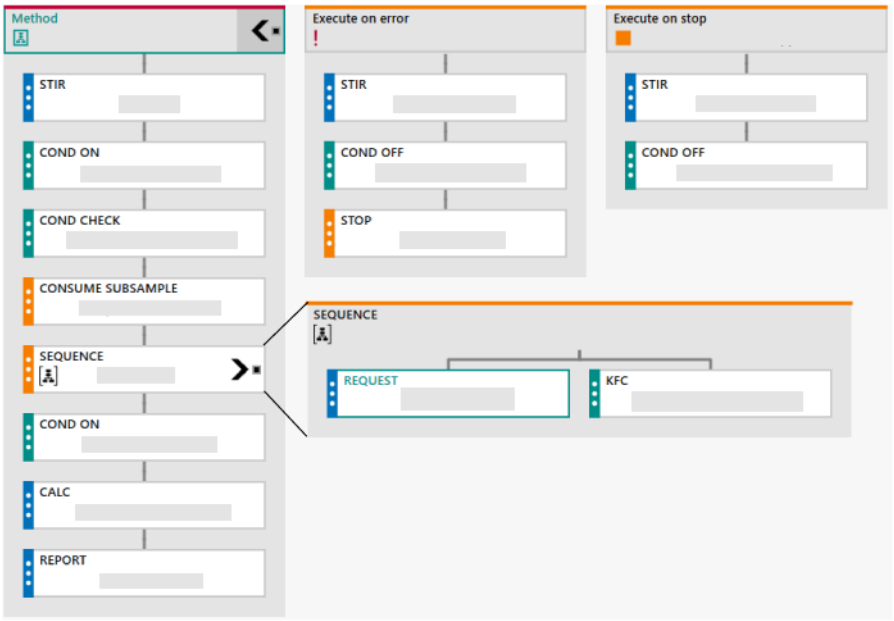
Karl Fischer titration coulometric – Run (chapter 5.11.8.11.1, page 594)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

5.11.8.11.1 Karl Fischer titration coulometric – Run

The **KFC** command can be executed with and without conditioning.
If conditioning is necessary, the conditioning commands **COND ON** (Start conditioning) and **COND CHECK** (Monitor conditioning) must be inserted before the **KFC** command.
If reconditioning is necessary, a **COND ON** command must be inserted in the method again after the **KFC** command.

A standard method for **KFC** with conditioning may look as follows:



The **KFC** command is executed in the following steps:

1 – Preconditioning

A KFC work system can be conditioned by adding a **COND ON** command and a **COND CHECK** command before the **KFC** command in the KF method.

The transition from conditioning to titration is defined in the **COND CHECK** command under **Titration start**. If **Manual / After sample addition** was selected, the titration can be started manually after conditioning with the **[Start titration]** button in the live data of the determination. Or the titration is automatically started at the recognition of a sample addition if the check box **Recognition of sample addition** is activated in the referenced titration command. If **Automatic after COND OK** was selected, the titration starts automatically as soon as the conditioning conditions **Start drift** and **Stabilizing time** of the referenced titration command are fulfilled and the **Sample addition time** has elapsed.

2 – Processing the start conditions

The **Pause** time is allowed to elapse before the actual titration is started.

3 – Carrying out the titration with the set control parameters and titration parameters

The titration is carried out according to the parameters defined under **Endpoint control parameters** and under **Titration parameters**.

- **Fixed point evaluation**
  Optionally, up to 9 fixed points can be defined in **Fixed point evaluation** that are calculated from the measuring point list during the titration.

- **Chart – … axes**
  Optionally, different quantities can be selected for the x-axis and y-axis. Display y2-axis can also be activated.

4 – Completing the titration

The titration is completed normally as soon as the endpoint and the stop criteria under Endpoint control parameters have been met.

The condition defined under **Stop conditions** is constantly monitored during the titration.

A running titration can be canceled by a manual cancellation or with the emergency stop or in case of an error.

5 – Reconditioning

A KFC work system can be conditioned further after the determination has ended (reconditioning) by inserting another **COND ON** command in the KF method at the end of a process run after a **KFC** command.

In doing so, the titration cell is conditioned even without a running sub-sample. Conditioning can be stopped manually in the window of the respective work system.

See also

COND CHECK – Command variables (chapter 5.11.8.15.1, page 608)

COND CHECK – Parameters (chapter 5.11.8.15, page 606)

COND OFF – Parameters (chapter 5.11.8.14, page 605)

COND ON – Parameters (chapter 5.11.8.13, page 604)

Conditioning – Principle (chapter 5.11.8.10, page 567)

KFC – Command variables (chapter 5.11.8.11.2, page 596)

KFC – Properties (chapter 5.11.8.11, page 586)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

5.11.8.11.2 KFC – Command variables

The following variables are generated by the **KFC** command during the process sequence and can be used as '**Variable name**.*Command name*' in a formula.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables

'**Amount.DriftCorrection**.'*Command name*'

Water quantity used to correct the water quantity at the endpoint. This is used when working with **Conditioning** and when **Automatic** or **Manual** has been selected for the **Correction with amount drift** parameter.

The correction water quantity is calculated by multiplying the amount drift with the time period from the end of conditioning until the end of the titration.

Unit: µg

'**Amount.EP{1}**.*Command name*'

Water quantity in the subsample at the endpoint.

Unit: µg

'**Amount.Final**.*Command name*'

Water quantity in the subsample after processing the command.

Unit: µg

'**Amount.FP{1}**.*Command name*'

Water quantity in the subsample at the fixed point.

Unit: µg

'**Charge.Final**.*Command name*'

Amount of charge for the last measuring point in the measuring point list.

Unit: mAs

'**Driftvalue.DriftCorrection**.*Command name*'

Amount drift that was used for correcting the EP water content.

When working with **Conditioning** this amount drift is used for calculating the correction of the EP water content if **Automatic** or **Manual** was selected for the **Correction with amount drift** parameter.

Unit: µg/min

'**Driftvalue.EP{1}**.*Command name*'

Amount drift at the endpoint.

Unit: µg/min

'**Driftvalue.Final**.*Command name*'

Amount drift for the last measuring point in the measuring point list.

Unit: µg/min

'**Duration**.*Command name*'

Total duration for the processing of the command.

Unit: s

'**Duration.DriftCorrection**.*Command name*'

Period from the end of conditioning until the end of the titration.

When working with **Conditioning**, this time period is used for calculating the correction of the EP volume if **Automatic** or **Manual** was selected for the **Correction with amount drift** parameter.

Unit: s

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**Index.EP{1}**.*Command name*'

Index of the endpoint.

Unit: None

'**Index.FP{1}**.*Command name*'

Index of the fixed point.

Unit: None

'**Measvalue.EP{1}**.*Command name*'

Measured value of the endpoint.

Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable

---

'**Measvalue.Final**.*Command name*'

End measured value after processing the command.

Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable

---

'**Measvalue.FP{1}**.*Command name*'

Measured value of the fixed point.

Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable

---

'**Temperature.EP{1}**.*Command name*'

Temperature associated with the endpoint.

Unit: °C

'**Temperature.Final**.*Command name*'

End temperature after processing the command.

Unit: °C

'**Temperature.FP{1}**.*Command name*'

Temperature associated with the fixed point.

Unit: °C

'**Time.EP{1}**.*Command name*'

Time stamp associated with the endpoint.

Unit: s

'**Time.Final**.*Command name*'

Time stamp for the last measuring point in the measuring point list.

Unit: s

'**Time.FP{1}**.*Command name*'

Time stamp associated with the fixed point.

Unit: s

'**Unit.Measvalue**.*Command name*'

Unit of the measured value.

Unit: mV

Equipment variables
'**Name.CurrentSensor**.*Command name*'
Name of the sensor used to measure the required measured quantity.

See also

Conditioning – Principle (chapter 5.11.8.10, page 567)

KFC – Properties (chapter 5.11.8.11, page 586)

Karl Fischer titration coulometric – Run (chapter 5.11.8.11.1, page 594)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

5.11.8.12 COLLECT – Concept

Structure

Measuring points from a primary command that generates measured values can be combined with at least one measured value from a secondary command using the **COLLECT** command. A measuring point list is saved during the run and the defined values from commands are displayed in the subsections **Live data** and **Curves**.

The **COLLECT** command can be inserted anywhere in methods and operating procedures. An incomplete or empty measuring point list may occur, however, depending on the placement. In order to generate a complete measuring point list, observe the following:

- When used within a method, the **COLLECT** command should run parallel to the primary command.

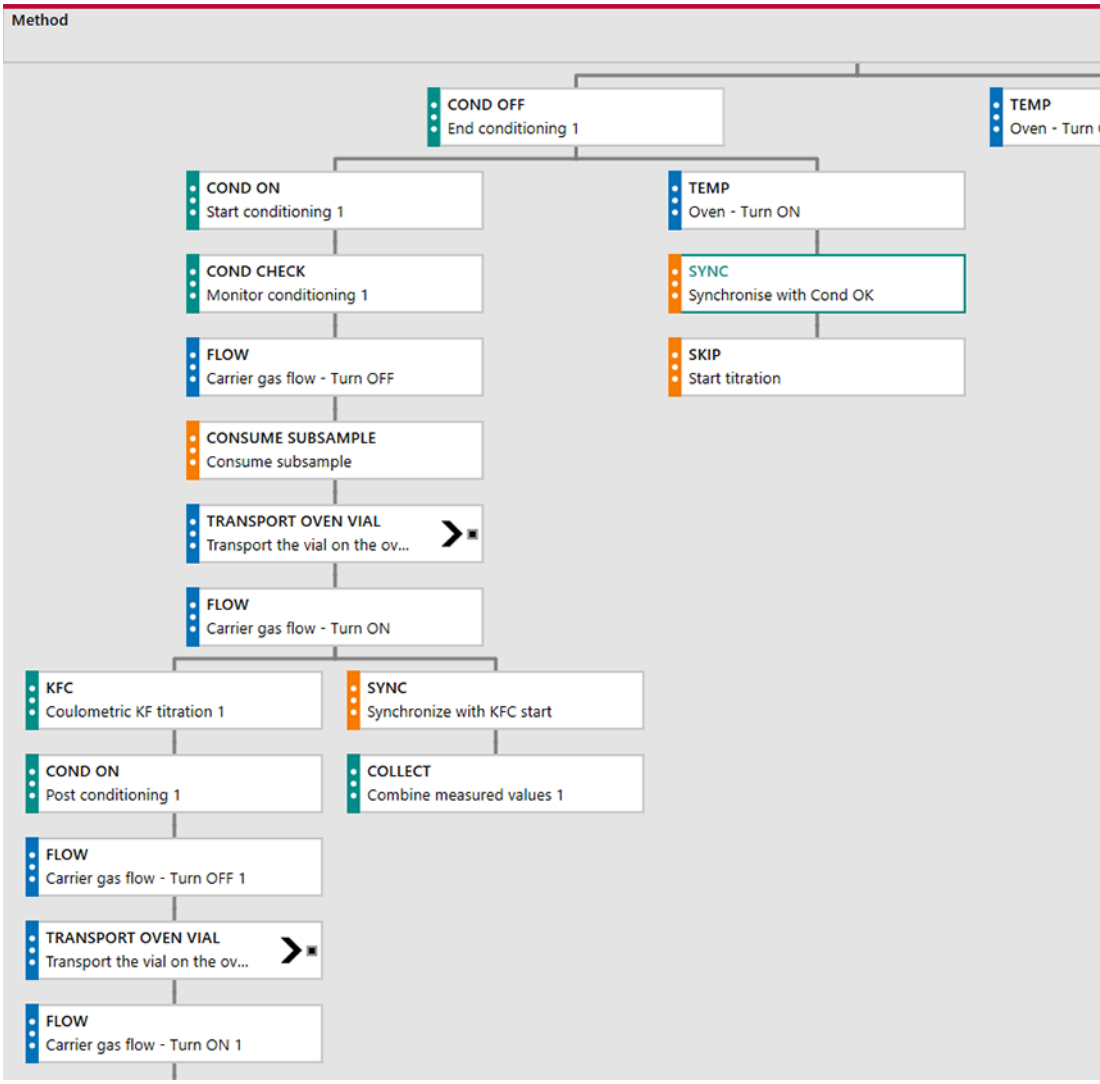
- When used within an operating procedure, the **COLLECT** command should run parallel to the first method of the operating procedure.

Arrangement in the method

In this example, a coulometric Karl Fischer titration is carried out with the **OMNIS Sample Robot Oven** sample robot for the automation section. In order to ensure that the **COLLECT** command does not start until after the primary command (KFC) has started, a **SYNC** command with the following condition is executed in parallel to the **KFC** command:

'**Finished**.*Coulometric KF titration 1*'' = 0, i.e. the **KFC** command is being executed.

In the **COLLECT** command, the **TEMP** *Oven – Turn ON* and **FLOW** *Carrier gas flow – Turn ON* commands are entered as secondary commands.

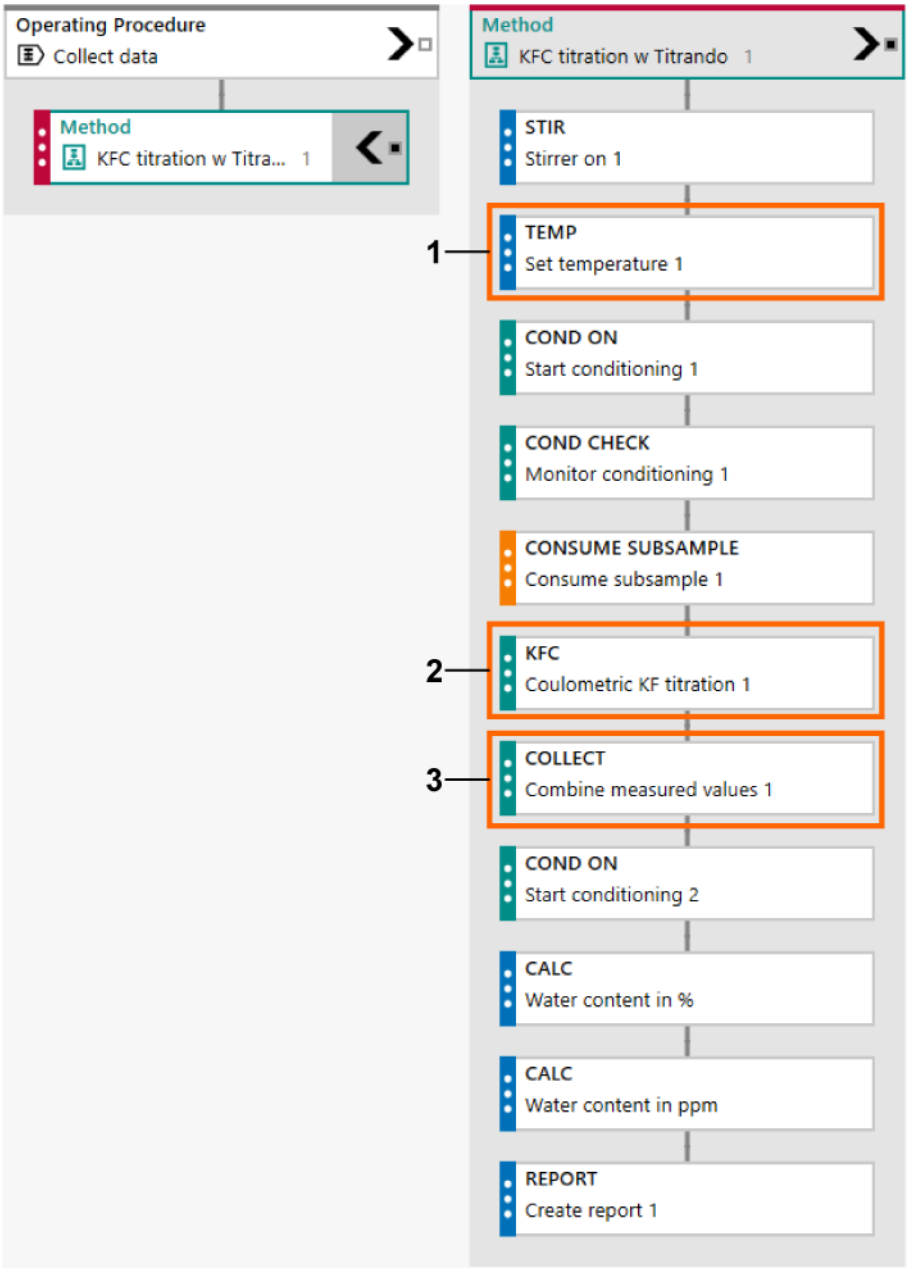


Incorrect arrangement

Possible causes for an incomplete or missing measuring point list:

- The **COLLECT** command is placed at the end of an operating procedure: The command is exited without creating a measuring point list.
- The **COLLECT** command does not start until the primary command has already run: The measuring points from the time period before the start of the **COLLECT** command are missing from the measuring point list of the **COLLECT** command.
- The secondary command is terminated before the start of the **COLLECT** command or begins later: The measured values from the secondary command are entered with **Invalid**.

The following example shows an arrangement of methods and commands within an operating procedure in which **no** measuring point list is created.



1. The secondary command **(1)** starts. No measuring point list is created.
2. The primary command **(2)** starts.
3.
4. The primary command is terminated before the **COLLECT** command **(3)** is started. No measuring point list is created because the primary command is no longer being executed.

See also

COLLECT – Parameters (chapter 5.11.8.12.1, page 602)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

5.11.8.12.1 COLLECT – Parameters

Measuring points from a primary command that generates measured values can be combined with at least one measured value from a secondary command using the **COLLECT** command. A measuring point list is saved during the run and the defined values from commands are displayed in the subsections **Live data** and **Curves**.

The **COLLECT** command should be inserted in the operating procedure parallel to the first method of the operating procedure so that a complete measuring point list can be created. If the **COLLECT** command is used within the method, the command must be placed before the primary command.

If the **COLLECT** command is placed incorrectly, the command can create no or only an incomplete list of measuring points.
Additional information on the **COLLECT** command: *(see "COLLECT – Concept", chapter 5.11.8.12, page 599)*

The **COLLECT** command is executed with the parameters listed in the following:

Commands	
Select primary command	Selection of the primary command. The recording of the measured values of the **COLLECT** command begins as soon as the primary command starts in the sequence of the operating procedure. The cycle of the measured value recording is determined by the primary command: Every time an entry is made in the measuring point list of the primary command, the current value of the secondary command (same value as in the **Live data**) is recorded in the **COLLECT** command. It is thus possible that the value of the secondary command in the measuring point list of the **COLLECT** command deviates from the value in the measuring point list of the secondary command. This field must not be left empty.
Add measured quantities	Selection of at least one secondary command. The measured quantities of the secondary commands are then available in the selection lists of the axes. Every measuring point of the primary command is supplemented by the measured values of the selected secondary commands. This field must not be left empty.

Titration commands, measuring commands and calibration commands from methods that are contained in the operating procedure are suggested in the selection list of the primary command.

The following commands are available in the selection list of the secondary commands: Titration commands, measuring commands and calibration commands as well as **TEMP**, **FLOW** and **ADD**. The commands originate from methods that are contained in the operating procedure.

In the case of methods in which the primary command leads to a **LOOP**, the first repetition of the primary command is used for the **COLLECT** command.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis. The selection list changes, depending on the selected primary command and the selected secondary commands. The default value of the primary command of the corresponding axis is applied as the default value for this axis.

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis. The selection list changes, depending on the selected primary command and the selected secondary commands. The default value of the primary command of the corresponding axis is applied as the default value for this axis.

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis. The selection list changes, depending on the selected primary command and the selected secondary commands. The default value of the primary command of the corresponding axis is applied as the default value for this axis.

The sequence of the columns in the measuring point list of the **COLLECT** command corresponds to the sequence defined in the **Add measured quantities** window.
If the same quantity was selected for multiple commands (e.g. temperature), then it can be seen in the measuring point list which quantity originates from which command.

See also

COLLECT – Concept (chapter 5.11.8.12, page 599)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

5.11.8.13 COND ON – Parameters

The **COND ON** command starts conditioning in endpoint titrations. The conditioning parameters can be defined in **Processes** ▶ **Method** ▶ **Properties** ▶ **Parameters** ▶ **Parameters for conditioning** for commands that support conditioning.

To use the **COND ON** command for reconditioning, it has to be added to the method after the titration command *(see "Karl Fischer titration – Principle", chapter 5.11.8.9, page 561), (see "Conditioning – Principle", chapter 5.11.8.10, page 567)(see "Conditioning – Principle", chapter 5.11.8.10, page 567)*.

The corresponding functional units of the referenced titration command are used to execute the **COND ON** command.
The **COND ON** command must be followed by a **COND CHECK** command to monitor the conditioning and show its progress.

The **COND ON** command is executed with the following parameters:

Referenced command	
Name of the titration command	Selection of the titration command for which the conditioning is carried out.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

COND CHECK – Parameters (chapter 5.11.8.15, page 606)

COND OFF – Parameters (chapter 5.11.8.14, page 605)

Command – Properties (chapter 5.11.8.1, page 431)

Conditioning – Principle (chapter 5.11.8.10, page 567)

Creating and editing a method (chapter 5.11.3.3, page 418)

KFC – Properties (chapter 5.11.8.11, page 586)

KFT – Command variables (chapter 5.11.8.10.3, page 582)

KFT – Properties (chapter 5.11.8.10.1, page 568)

Karl Fischer titration coulometric – Run (chapter 5.11.8.11.1, page 594)

Karl Fischer titration volumetric – Run (chapter 5.11.8.10.2, page 580)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

5.11.8.14 COND OFF – Parameters

The **COND OFF** command stops the conditioning and deactivates the polarization of the electrode (e.g. in case of an error).

The corresponding functional units of the referenced titration command are used to execute the **COND OFF** command.

The **COND OFF** command is executed with the following parameters:

Referenced command	
Name of the titration command	Selection of the titration command for which the conditioning is carried out.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

COND ON – Parameters (chapter 5.11.8.13, page 604)

Command – Properties (chapter 5.11.8.1, page 431)

Conditioning – Principle (chapter 5.11.8.10, page 567)

Creating and editing a method (chapter 5.11.3.3, page 418)

KFC – Properties (chapter 5.11.8.11, page 586)

KFT – Command variables (chapter 5.11.8.10.3, page 582)

KFT – Properties (chapter 5.11.8.10.1, page 568)

Karl Fischer titration coulometric – Run (chapter 5.11.8.11.1, page 594)

Karl Fischer titration volumetric – Run (chapter 5.11.8.10.2, page 580)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

5.11.8.15 COND CHECK – Parameters

Conditioning is monitored according to the parameters set in the referenced command with the **COND CHECK** command. In addition, the measured values during conditioning, the drift stability, the conditioning status and the curve are displayed with the **COND CHECK** command in the live display.

The determination can be paused manually during the execution of a **COND CHECK** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

The corresponding functional units of the referenced titration command are used to execute the **COND CHECK** command.
The **COND CHECK** command can only be executed if the conditioning was started earlier with a **COND ON** command.

The **COND CHECK** command is executed with the parameters listed in the following:

Referenced command	
Name of the titration command	Selection of the titration command for which the conditioning is carried out.

Titration start	
Titration start	The following titration can be started as follows: ▪ **Manual / After sample addition** The titration can be started manually with the **[Start titration]** button in the live data of the determination. or The titration is automatically started at the recognition of a sample addition if the check box **Recognition of sample addition** is activated in the respective titration command *(see "KFT – Properties", chapter 5.11.8.10.1, page 568)*. The **Recognition of sample addition** function is only available for the **KFC** command and the **KFT Ipol** command and only for OMNIS instruments. ▪ **Automatic after COND OK** The titration is automatically started as soon as the conditioning conditions Start drift und Stabilizing time of the referenced titration command are fulfilled and the Sample addition time has elapsed.

Recording of measured value	
Duration	With this parameter, the duration of the measured value recording during conditioning can be defined. Only the set time period in the past is displayed and saved at the end of the conditioning in the measuring point list and in the curve.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

CAL COND – Properties (chapter 5.11.8.34, page 695)

Commands – Definition (chapter 5.11.8, page 429)

Conditioning – Principle (chapter 5.11.8.10, page 567)

Creating and editing a method (chapter 5.11.3.3, page 418)

KFC – Properties (chapter 5.11.8.11, page 586)

KFT – Properties (chapter 5.11.8.10.1, page 568)

Karl Fischer titration coulometric – Run (chapter 5.11.8.11.1, page 594)

Karl Fischer titration volumetric – Run (chapter 5.11.8.10.2, page 580)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

MEAS COND – Properties (chapter 5.11.8.25, page 641)

SET – Properties (chapter 5.11.8.6.1, page 512)

SET – Run (chapter 5.11.8.6.2, page 527)

5.11.8.15.1 COND CHECK – Command variables

The following variables are generated by the **COND CHECK** command during the process sequence and can be used as '**Variable name**.*Command name*' under the **Command variables** variable category in a formula.

General variables

'**ConditioningStateOk**.*Command name*'

Status of the conditioning.

- **0**: Conditioning not OK
- **1**: Conditioning OK

'**Duration**.*Command name*'

Duration of the **COND CHECK** command.

Unit: s

'**Duration.Conditioning**.*Command name*'

Duration of the conditioning, i.e. from the start of the **COND ON** command until the end of the **COND CHECK** command.

When working with **Recognition of sample addition**, this value is corrected by the time **Time.SampleDetectOffset**.'*Command name*'.

Unit: s

'**Driftvalue.Conditioning**.*Command name*'

For the **KFC** command:

If the **Recognition of sample addition** is activated, this value corresponds to the amount drift prior to sample addition.

In all other cases, this value corresponds to the last amount drift from the **COND CHECK** command.

When working with **Conditioning**, this amount drift is used for calculating the EP water content correction if the **Correction with amount drift** parameter was activated with **Automatic**.

Unit: µg/min

For the **KFT** command and the **SET Ipol** command:

If the **Recognition of sample addition** is activated, this value corresponds to the volume drift prior to sample addition (only **KFT** command).

In all other cases, this value corresponds to the last volume drift from the **COND CHECK** command.

When working with **Conditioning**, this volume drift is used for calculating the EP volume correction if the **Correction with volume drift** parameter was activated with **Automatic**.

Unit: µL/min

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**Measvalue.Final**.*Command name*'

End measured value of the conditioning.

Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable

'**Time.SampleDetectOffset**.*Command name*'

Time that has elapsed since sample addition until it was recognized.

Unit: s

'**Unit.Measvalue**.*Command name*'

Unit for the variable '**Measvalue.Final**.*Command name*'

Variables for the KFC command

Command variables
'**Amount.Conditioning**.*Command name*' Water content of the subsample determined during conditioning. If the **Recognition of sample addition** is activated, then this value corresponds to the last value before the EP criterion was exceeded. In all other cases, this value corresponds to the last value from the measuring point list. Unit: µg
'**Amount.Final**.*Command name*' Water quantity at the end of the **COND CHECK** command. Unit: µg
'**Amount.SampleDetectOffset**.*Command name*' Water quantity that was titrated between the sample addition and its detection. Unit: µg

Variables for the KFT command and the SET Ipol command

Command variables
'**Volume.Conditioning**.*Command name*' Total dosed titrant volume for conditioning. When working with **Recognition of sample addition**, this value is corrected by the volume **Volume.SampleDetectOffset**.'*Command name*' (only **KFT** command). Unit: mL
'**Volume.Final**.*Command name*' Dosed titrant volume at the end of the **COND CHECK** command. Unit: mL
'**Volume.SampleDetectOffset**.*Command name*' (only **KFT** command) Volume that was dosed since sample addition until it was recognized. Unit: mL

See also

COND CHECK – Parameters (chapter 5.11.8.15, page 606)

Conditioning – Principle (chapter 5.11.8.10, page 567)

KFC – Command variables (chapter 5.11.8.11.2, page 596)

KFC – Properties (chapter 5.11.8.11, page 586)

KFT – Command variables (chapter 5.11.8.10.3, page 582)

KFT – Properties (chapter 5.11.8.10.1, page 568)

Karl Fischer titration coulometric – Run (chapter 5.11.8.11.1, page 594)

Karl Fischer titration volumetric – Run (chapter 5.11.8.10.2, page 580)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

SET – Command variables (chapter 5.11.8.6.3, page 530)

SET – Properties (chapter 5.11.8.6.1, page 512)

SET – Run (chapter 5.11.8.6.2, page 527)

5.11.8.16 PREDICT – Parameters

The **PREDICT** command is used to evaluate a measured spectrum based on a model or a model hierarchy. If a quantification model was used for the evaluation, then a slope/y-intercept correction can be applied if required.

The **PREDICT** command is executed with the following parameters:

Name of the measuring command	Select the name of the **MEAS SPEC** command with which the spectrum is acquired.

Structure	Use **Single model** or **Model hierarchy** for the evaluation of the spectrum.
Model type (If **Single model** was previously selected)	Select **Quantification model** or **Identification model**.
Quantification model	Select the quantification model to be used for the evaluation of a spectrum. Only the last published versions of the quantification models are displayed. **Optional**: Select the **Slope/y-intercept correction** that is to be applied to the results of the quantification model.
Identification model	Select the identification model to be used for the evaluation of a spectrum. Only the latest published versions of the identification models are displayed.
Model hierarchy	Select the model hierarchy that is to be used for the evaluation of a spectrum. Only the latest published versions of the model hierarchies are displayed.
Use for the verification (If **Identification model** or **Model hierarchy** was previously selected)	The selected identification model or the selected model hierarchy is used for verification.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

Models – Definition (chapter 5.13.1.1, page 1056)

PREDICT – Command variables (chapter 5.11.8.16.1, page 611)

Slope/y-intercept correction – Definition (chapter 5.13.2.6, page 1124)

5.11.8.16.1 PREDICT – Command variables

The following variables are generated by the **PREDICT** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

- Variables for selecting the quantification model type: *Variables of the quantification model type*
- Variables for selecting the identification model or model hierarchy model type: *Variables of the identification model or model hierarchy model type*

Variables of the quantification model type

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**IsOutlier.OutlierDetection.Result**.*Command name*' Rating of the predicted result as an outlier. ▪ **0**: The result is **not** an outlier. ▪ **1**: The result is an outlier.
'**HotellingsT2.OutlierDetection.Result**.*Command name*' Calculated result value (Hotelling's T²).
'**QResiduals.OutlierDetection.Result**.*Command name*' Calculated result value (Q residuals).
'**NearestNeighborDistance.OutlierDetection.Result.**.*Command name*' Calculated result value (Nearest Neighbor Distance).
'**Predicted.Quantification.Result**.*Command name*' Predicted end value. If a slope/y-intercept correction is used, the result will be corrected with this. Unit: Defined in the 'Unit.Result' variable
'**Unit.Quantification.Result**.*Command name*' Unit of the result. The unit is defined by the user in the properties of the referenced quantification model under **Models** ▶ **Quantification models** ▶ **Spectra list** in the **Reference parameter / unit** field.
'**Uncorrected.Quantification.Result**.*Command name*' Result value of the evaluation of a spectrum without the use of a slope/y-intercept correction. Unit: Defined in the 'Unit.Result' variable
'**LimitHotellingsT2.OutlierDetection.Result**.*Command name*' Limit value of the (Hotelling's T²) outliers.
'**LimitQResiduals.OutlierDetection.Result**.*Command name*' Limit value of the (Q residuals) outliers.

Command variables
'**LimitNearestNeighborDistance.OutlierDetection.Result.**.*Command name*' Calculated NND limit.

Variables of the "Identification model" model type

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Probability.Identification.Result**.*Command name*' ▪ **Invalid**: The identification of the product or product group has failed. ▪ **0.01–100**: The probability in percent that the analyzed spectrum is the identified product or product group.
'**Status.Identification.Result**.*Command name*' ▪ **Ambiguous**: The identification of the product or product group has failed. No product or product group has been unambiguously identified. ▪ **Not identified**: The identification of the product or product group has failed. No product or product group has been identified. ▪ **Identified**: The product or product group has been successfully identified. A product or product group has been identified.
'**Product.Identification.Result**.*Command name*' ▪ ***Product name*** or ***Name of the product group***: Name of the identified product or product group. If the identification of the product or the product group has failed, then no result will be displayed.
'**Status.Verification.Result**.*Command name*' ▪ **0**: The verification of the product has failed. The product has not been verified. ▪ **1**: The verification of the product is successful. The product has been verified. **Note:** This variable is available only if the identification model was used for verification.

Variables of the model hierarchy

In the following variables, the index of the quantification models does not refer globally to the entire model hierarchy.

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Probability.Identification.Result**.*Command name*' ▪ **Invalid**: The identification of the product or product group has failed. ▪ **0.01–100**: The probability in percent that the analyzed spectrum is the identified product or product group.
'**Status.Identification.Result**.*Command name*' ▪ **Ambiguous**: The identification of the product or product group has failed. No product or product group has been unambiguously identified. ▪ **Not identified**: The identification of the product or product group has failed. No product or product group has been identified. ▪ **Identified**: The product or product group has been successfully identified. A product or product group has been identified.
'**Product.Identification.Result**.*Command name*' ▪ ***Product name*** or ***Name of the product group***: Name of the identified product or product group. If the identification of the product or the product group has failed, then no result will be displayed.
'**IsOutlier.OutlierDetection{x}.Result**.*Command name*' (x = index of the quantification model, Default value = 1) Rating of the predicted result as an outlier. ▪ **0**: The result is **not** an outlier. ▪ **1**: The result is an outlier.
'**AnyOutlier.OutlierDetection.Result**.*Command name*' Status of the outliers of the quantification models in the model hierarchy: ▪ **0**: The quantification models of the model hierarchy does not contain any outliers. ▪ **1**: The quantification models of the model hierarchy contains outliers.
'**ParameterName.Quantification{x}.Result.**.*Command name*' (x = index of the quantification model, Default value = 1) Name of the reference parameter.
'**HotellingsT2.OutlierDetection{x}.Result**.*Command name*' (x = index of the quantification model, Default value = 1) Calculated result value (Hotelling's T^2).

Command variables
'**LimitHotellingsT2.OutlierDetection{x}.Result**.*Command name*' (x = index of the quantification model, Default value = 1) Limit value of the (Hotelling's T²) outliers.
'**QResiduals.OutlierDetection{x}.Result**.*Command name*' (x = index of the quantification model, Default value = 1) Calculated result value (Q residuals).
'**LimitQResiduals.OutlierDetection{x}.Result**.*Command name*' (x = index of the quantification model, Default value = 1) Limit value of the (Q residuals) outliers.
'**NearestNeighborDistance.OutlierDetection{x}.Result.**.*Command name*' (x = index of the quantification model, Default value = 1) Calculated result value (Nearest Neighbor Distance).
'**LimitNearestNeighborDistance.OutlierDetection{x}.Result.**.*Command name*' (x = index of the quantification model, Default value = 1) Calculated NND limit.
'**Predicted.Quantification{x}.Result**.*Command name*' (x = index of the quantification model, Default value = 1) Predicted end value. If a slope/y-intercept correction is used, the result will be corrected with this. Unit: Defined in the 'Unit.Result' variable
'**Unit.Quantification{x}.Result**.*Command name*' (x = index of the quantification model, Default value = 1) Unit of the result. The unit is defined by the user in the properties of the referenced quantification model under **Models** ▶ **Quantification models** ▶ **Spectra list** in the **Reference parameter / unit** field.
'**Uncorrected.Quantification{x}.Result**.*Command name*' (x = index of the quantification model, Default value = 1) Result value of the evaluation of a spectrum without the use of a slope/y-intercept correction. Unit: Defined in the 'Unit.Result' variable
'**Status.Verification.Result**.*Command name*' ▪ **0**: The verification of the product has failed. The product has not been verified. ▪ **1**: The verification of the product is successful. The product has been verified. **Note:** This variable is available only if the model hierarchy was used for verification.

See also

PREDICT – Parameters (chapter 5.11.8.16, page 610)

5.11.8.17 VAL WL – Properties

The **VAL WL** command is used to validate the wavelength calibration of the spectrometer which was carried out with the **CAL WL** command.

After selecting the **VAL WL** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **VAL WL** command:

Parameters

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Wavelength** (default value) ▪ **Absorbance**
Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Wavelength** ▪ **Absorbance** (default value)
Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Wavelength** ▪ **Absorbance** (default value)

All events and actions that affect the **VAL WL** command and are executed in the OMNIS Software are recorded in the **Audit Trail** work area.

Execute with

In order for a **VAL WL** command to be executed, an instrument of the **2060 The NIR** type or a functional unit of the **Liquid Sample Presentation** type or of the **Solid Sample Presentation** type needs to be assigned to the command.

See also

CAL WL – Command variables (chapter 5.11.8.21.1, page 627)

CAL WL – Properties (chapter 5.11.8.21, page 626)

Creating and editing a method (chapter 5.11.3.3, page 418)

VAL WL – Command variables (chapter 5.11.8.17.1, page 617)

5.11.8.17.1 VAL WL – Command variables

The following variables are generated by the **VAL WL** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Date.Result**.*Command name*' Time when the wavelength calibration was validated.
'**ExpectedBandwidth.Peak{}**.*Command name*' Expected bandwidth of the defined peak. Unit: nm
'**ExpectedWavelength.Peak{}**.*Command name*' Expected wavelength of the defined peak. Unit: nm
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Index.Peak{}**.*Command name*' Index of the peak.
'**MeasuredBandwidth.Peak{}**.*Command name*' Measured bandwidth of the defined peak. Unit: nm
'**MeasuredWavelength.Peak{}**.*Command name*' Measured wavelength of the defined peak. Unit: nm

Command variables
'**OverallStatus.Result**.*Command name*' Overall validation status of the validation of the wavelength calibration. ▪ **1**: The validation was successful. ▪ **2**: The validation failed.

See also

CAL WL – Command variables (chapter 5.11.8.21.1, page 627)

CAL WL – Properties (chapter 5.11.8.21, page 626)

VAL WL – Properties (chapter 5.11.8.17, page 616)

5.11.8.18 VAL REF STD – Properties

The **VAL REF STD** command is used to validate the absorbance values on specific wavelength ranges with the values determined in the reference standardization (**REF STD** command).

After selecting the **VAL REF STD** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **VAL REF STD** command:

Parameters

Measuring parameters	
Channel	Selection of the channel for which the reference standardization is validated.
Interface	Selection of the interface that is used to validate the reference standardization. ▪ **Fiber optic**: The reference standardization is validated via a fiber optic interface in the reflection mode or the transmission mode. ▪ **Window**: The reference standardization is validated via a different interface than for the fiber optic correction or via a glass window.

Measuring parameters	
Measuring mode	Selection of the measuring mode in which the reference standardization is validated. ▪ **Reflection**: The reference standardization is validated in the reflection mode. Reflection measurements are carried out with NIR reflection standards. The light that is reflected by the standard is measured. If **Reflection** is selected, then the following specific parameter appears: – Reflection standard ▪ **Transmission**: The reference standardization is validated in the transmission mode. Transmission measurements are performed on transparent samples. The light that directly goes through the sample (along the optical axis) is determined.
Reflection standard	Selection of the external NIR reflection standard that is used for the validation of the reference standardization. Additional information on the standards: *(see "Standards – Subsection", chapter 5.12.11, page 1050)*, *(see "Importing standards", chapter 5.12.11.2, page 1053)*

3 spectra are recorded per **VAL REF STD** command: Measured corrected spectrum, Reference spectrum and Validation residuals.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Wavelength** (default value) ▪ **Absorbance** To display **Absorbance** on the x-axis, one of the following 3 options must be selected: – **Measured corrected spectrum** – **Reference spectrum** – **Validation residuals**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Wavelength** ▪ **Absorbance** To display **Absorbance** on the y-axis, one of the following 3 options must be selected: – **Measured corrected spectrum** – **Reference spectrum** – **Validation residuals** (default value)

Chart – y2-axis	
Display y2-axis	Display of a 2nd y-axis for displaying another quantity as a curve.
Quantity	Selection of the specified quantity to be shown in the curve display on the 2nd y-axis: ▪ **Wavelength** ▪ **Absorbance** To display **Absorbance** on the second y-axis, one of the following 3 options must be selected: – **Measured corrected spectrum** (default value) – **Reference spectrum** – **Validation residuals**

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

All events and actions that affect the **VAL REF STD** command and are executed in the OMNIS Software are recorded in the **Audit Trail** work area.

Execute with

For a **VAL REF STD** command to be executed, an instrument of the **2060 The NIR** type must be assigned.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

Importing standards (chapter 5.12.11.2, page 1053)

REF STD – Command variables (chapter 5.11.8.19.1, page 623)

REF STD – Properties (chapter 5.11.8.19, page 621)

Standards – Properties (chapter 5.12.11.1, page 1052)

VAL REF STD – Command variables (chapter 5.11.8.18.1, page 620)

5.11.8.18.1 VAL REF STD – Command variables

The following variables are generated by the **VAL REF STD** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Date.Result**.*Command name*' Time at which the reference standardization was validated.

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**OverallStatus.Result**.*Command name*' Overall validation status of the reference standardization. ▪ **1**: The validation was successful. ▪ **2**: The validation failed.

See also

REF STD – Command variables (chapter 5.11.8.19.1, page 623)

REF STD – Properties (chapter 5.11.8.19, page 621)

VAL REF STD – Properties (chapter 5.11.8.18, page 618)

5.11.8.19 REF STD – Properties

The **REF STD** command is used to remove interferences of optical fibers and measuring probes from the absorption spectrum of the sample. Reference standardization ensures that absorbance values on a certain wavelength range are comparable between different systems.

After selecting the **REF STD** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **REF STD** command:

Parameters

Measuring parameters	
Channel	Selection of the channel for which the reference standardization is executed.

Measuring parameters	
Interface	Selection of the interface that is used to execute the reference standardization. ▪ **Fiber optic**: The reference standardization is executed via a fiber optic in the reflection mode or the transmission mode. ▪ **Window**: The reference standardization is performed via a different interface than for the fiber optic correction or via a glass window.
Measuring mode	Selection of the measuring mode in which the reference standardization is executed. ▪ **Reflection**: The reference standardization is executed in the reflection mode. Reflection measurements are carried out with NIR reflection standards. The light that is reflected by the standard is measured. If **Reflection** is selected, the following specific parameter appears: – **Reflection standard** ▪ **Transmission**: The reference standardization is executed in the transmission mode. Transmission measurements are performed through air. The light that directly goes through the sample (along the optical axis) is measured.
Reflection standard	Selection of the external NIR reflection standard that is used for the reference standardization. Additional information on the standards: *(see "Standards – Subsection", chapter 5.12.11, page 1050)*, *(see "Importing standards", chapter 5.12.11.2, page 1053)*

3 spectra are recorded per **REF STD** command: Measured raw spectrum, Reference spectrum and Correction spectrum.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Wavelength** (default value) ▪ **Absorbance** To display **Absorbance** on the x-axis, one of the following 3 options must be selected: – **Measured raw spectrum** – **Reference spectrum** – **Correction spectrum**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Wavelength** ▪ **Absorbance** To display **Absorbance** on the y-axis, one of the following 3 options must be selected: – **Measured raw spectrum** – **Reference spectrum** – **Correction spectrum** (default value)

Chart – y2-axis	
Display y2-axis	Display of a 2nd y-axis for displaying another quantity as a curve.
Quantity	Selection of the specified quantity to be shown in the curve display on the 2nd y-axis: ▪ **Wavelength** ▪ **Absorbance** To display **Absorbance** on the second y-axis, one of the following 3 options must be selected: – **Measured raw spectrum** (default value) – **Reference spectrum** – **Correction spectrum**

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

For a **REF STD** command to be executed, an instrument of the **2060 The NIR** type must be assigned.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

Importing standards (chapter 5.12.11.2, page 1053)

REF STD – Command variables (chapter 5.11.8.19.1, page 623)

Standards – Properties (chapter 5.12.11.1, page 1052)

VAL REF STD – Command variables (chapter 5.11.8.18.1, page 620)

VAL REF STD – Properties (chapter 5.11.8.18, page 618)

5.11.8.19.1 REF STD – Command variables

The following variables are generated by the **REF STD** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Date.Result**.*Command name*' Time at which the reference standardization was executed.
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

See also

REF STD – Properties (chapter 5.11.8.19, page 621)

VAL REF STD – Command variables (chapter 5.11.8.18.1, page 620)

VAL REF STD – Properties (chapter 5.11.8.18, page 618)

5.11.8.20 MEAS REF SPEC – Properties

The **MEAS REF SPEC** command is used to record the reference spectrum for the measurement of samples.

After selecting the **MEAS REF SPEC** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS REF SPEC** command:

Parameters

The following parameters apply only for instruments of the **2060 The NIR** type.

Integration time	Selection of the type of integration time determination. ▪ **Automatic**: The integration time is determined automatically by the instrument. ▪ **Manual**: The integration time is defined manually. If **Manual** is selected, the following specific parameter appears: – **Integration time**.

Integration time	A higher integration time improves the signal-to-noise ratio. Integration times that are too high lead to a saturation of the detector which means that the spectra cannot be evaluated anymore.
Averaged spectra	Number of spectra to be used for the formation of the mean spectrum of a subsample. A high number of spectra improves the signal-to-noise ratio. The higher the number of spectra, the longer the measurement takes.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **MEAS REF SPEC** command to be executed, an instrument of the **2060 The NIR** type or a functional unit of the **Liquid Sample Presentation** type or of the **Solid Sample Presentation** type needs to be assigned to the command.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS REF SPEC – Command variables (chapter 5.11.8.20.1, page 625)

MEAS SPEC – Command variables (chapter 5.11.8.31.1, page 678)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

5.11.8.20.1 MEAS REF SPEC – Command variables

The following variables are generated by the **MEAS REF SPEC** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Date.Result**.*Command name*' Time at which the reference spectrum was acquired.
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

The following variables are additionally available if a functional unit of the **Liquid Sample Presentation** type was assigned to the command beforehand in **Properties** ▶ **Execute with**.

Table 5

'**TemperatureControlMode.Result**.*Command name*' Place of temperature control ▪ **Inactive**: No temperature control. ▪ **Sample holder**: The temperature was controlled on the sample holder. ▪ **Sample vessel**: The temperature was controlled on the sample vessel.
'**CurrentTemperature.Result**.*Command name*' Current temperature while the command is being executed. Unit: °C

See also

MEAS REF SPEC – Properties (chapter 5.11.8.20, page 624)

5.11.8.21 CAL WL – Properties

The **CAL WL** command is used to carry out a wavelength calibration. For this, each pixel of the spectrometer is assigned a wavelength.

After selecting the **CAL WL** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **CAL WL** command:

Parameters

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Wavelength** (default value) ▪ **Absorbance**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Wavelength** ▪ **Absorbance** (default value)

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Wavelength** ▪ **Absorbance** (default value)

Execute with

In order for a **CAL WL** command to be executed, an instrument of the **2060 The NIR** type or a functional unit of the **Liquid Sample Presentation** type or of the **Solid Sample Presentation** type needs to be assigned to the command.

See also

CAL WL – Command variables (chapter 5.11.8.21.1, page 627)

Creating and editing a method (chapter 5.11.3.3, page 418)

VAL WL – Command variables (chapter 5.11.8.17.1, page 617)

VAL WL – Properties (chapter 5.11.8.17, page 616)

5.11.8.21.1 CAL WL – Command variables

The following variables are generated by the **CAL WL** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Date.Result**.*Command name*' Time at which the wavelength calibration was carried out.
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

See also

CAL WL – Properties (chapter 5.11.8.21, page 626)

VAL WL – Command variables (chapter 5.11.8.17.1, page 617)

VAL WL – Properties (chapter 5.11.8.17, page 616)

5.11.8.22 TEST NOISE – Properties

The **TEST NOISE** command is used to test the signal noise of the spectrometer. The photometric noise, the peak-to-peak noise, and the baseline bias of 10 spectra in different segments are determined and compared to the tolerance values.

After selecting the **TEST NOISE** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **TEST NOISE** command:

Parameters

Measuring parameters **(only for instruments of the 2060 The NIR type)**	
Measuring mode	Selection of the measuring mode used to check the signal noise. ▪ **Internal**: The signal noise of the spectrometer is tested via a reference channel. ▪ **External transmission**: The signal noise of the sample channel is tested in transmission mode via a connected measuring channel. If **External transmission** is selected, the following parameter appears: – **Channel** ▪ **External reflection**: The signal noise of the sample channel is tested in reflection mode via a connected measuring channel. Reflection measurements are carried out with NIR reflection standards. The light that is reflected by the standard is measured. If **External reflection** is selected, the following parameters appear: – **Channel**, **Reflection standard** **Note**: Different tolerances are applied, depending on the selected measuring mode.
Channel	Selection of the measuring channel in which the noise is tested.
Reflection standard	Selection of the external reflection standard that is used for testing of the signal noise. Additional information on the standards: *(see "Standards – Subsection", chapter 5.12.11, page 1050)*, *(see "Importing standards", chapter 5.12.11.2, page 1053)*

10 spectra are recorded per **TEST NOISE** command.

Chart – x-axis	
Quantity	Selection of the specified quantity or absorbance to be shown in the curve display on the x-axis: ▪ **Wavelength** ▪ **Spectrum 1–Spectrum 10**

Chart – y-axis	
Quantity	Selection of the specified quantity or absorbance to be shown in the curve display on the y-axis: ▪ **Wavelength** ▪ **Spectrum 1–Spectrum 10**

Chart – y2-axis	
Display y2-axis	Display of a 2nd y-axis for displaying another quantity as a curve.
Quantity	Selection of the specified quantity or absorbance to be shown in the curve display on the 2nd y-axis: ▪ **Wavelength** ▪ **Spectrum 1–Spectrum 10**

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

All events and actions that affect the **TEST NOISE** command and are executed in the OMNIS Software are recorded in the **Audit Trail** work area.

Execute with

In order for a **TEST NOISE** command to be executed, an instrument of the **2060 The NIR** type or a functional unit of the **Liquid Sample Presentation** type or of the **Solid Sample Presentation** type needs to be assigned to the command.

See also

CAL WL – Properties (chapter 5.11.8.21, page 626)

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS REF SPEC – Properties (chapter 5.11.8.20, page 624)

Standards – Subsection (chapter 5.12.11, page 1050)

TEST NOISE – Command variables (chapter 5.11.8.22.1, page 630)

TEST WL – Properties (chapter 5.11.8.23, page 630)

VAL WL – Properties (chapter 5.11.8.17, page 616)

5.11.8.22.1 TEST NOISE – Command variables

The following variables are generated by the **TEST NOISE** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Date.Result**.*Command name*' Time at which the signal noise was tested.
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**OverallStatus.Result**.*Command name*' Overall validation status of the test. ▪ **1**: The validation was successful. ▪ **2**: The validation failed.

See also

TEST NOISE – Properties (chapter 5.11.8.22, page 628)

5.11.8.23 TEST WL – Properties

The **TEST WL** command is used to check the wavelength accuracy of the spectrometer. An internal wavelength standard is measured 10 times. Peak positions are determined, statistically evaluated, and compared with set-point values at this time.

After selecting the **TEST WL** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **TEST WL** command:

Parameters

Measuring parameters (only for instruments of the 2060 The NIR type)	
Measuring mode	Selection of the measuring mode for the test of the wavelength accuracy. ▪ **Internal**: The wavelength accuracy of the spectrometer is tested via a reference channel. ▪ **External**: The wavelength accuracy of the sample channel is tested via a connected measuring channel. If **External** is selected, then the following specific parameter appears: – **Channel**
Channel	Selection of the measuring channel in which the spectra are acquired.

Measuring parameters (only functional units of the Liquid Sample Presentation type)	
Measuring mode	Selection of the wavelength filter for the test of the wavelength accuracy. ▪ **Internal**: The wavelength accuracy of the spectrometer is tested via the internal wavelength standard. ▪ **External**: The wavelength accuracy is tested in the sample position via an external wavelength standard. If **External** is selected, then the following specific parameter appears: – **Transmission standard**
Transmission standard	Selection of the external transmission standard.

Measuring parameters (only functional units of the Solid Sample Presentation type)	
Measuring mode	Selection of the wavelength filter for the test of the wavelength accuracy. ▪ **Internal**: The wavelength accuracy of the spectrometer is tested via the internal wavelength standard. ▪ **External**: The wavelength accuracy is tested in the sample position via an external wavelength standard. If **External** is selected, then the following specific parameter appears: – **Reflection standard**
Reflection standard	Selection of the external reflection standard.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

All events and actions that affect the **TEST WL** command and are executed in the OMNIS Software are recorded in the **Audit Trail** work area.

Execute with

In order for a **TEST WL** command to be executed, an instrument of the **2060 The NIR** type or a functional unit of the **Liquid Sample Presentation** type or of the **Solid Sample Presentation** type needs to be assigned to the command.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

TEST WL – Command variables (chapter 5.11.8.23.1, page 632)

5.11.8.23.1 TEST WL – Command variables

The following variables are generated by the **TEST WL** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Date.Result**.*Command name*' Time at which the test of the wavelength accuracy was carried out.
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**OverallStatus.Result**.*Command name*' Overall status of the test of the wavelength accuracy. ▪ **1**: The test was successful. ▪ **2**: The test failed.

See also

TEST WL – Properties (chapter 5.11.8.23, page 630)

5.11.8.24 Temperature control and sample processing – principle

Temperature control on the spectrometer can be managed not only in the sample holder but also in the sample vessel of the liquid sample presentation. The user can select whether the temperature of the sample holder or the temperature of the sample is to be controlled. It is also possible to completely deactivate the temperature control. The **PREP SPEC** command is used to set the temperature control and to select the sample vessel with the corresponding sample holder.

The temperature control in the sample is supported for the following sample vessel types: **Disposable vial 2 mm (67402070), Disposable vial 4 mm (67402250), Disposable vial 8 mm (67402240), Disposable vial 10 mm (67402100)**.

The temperature control in the sample is **not** supported for sample vessels of the **Flow-through cell** and **Cuvette** types. Only the temperature control in the sample holder is available for sample vessels of the **Flow-through cell** and **Cuvette** types.

The temperature control in the sample was validated, based on various criteria:

- Target temperature of the sample: between 25 °C and 80 °C.
- Accuracy ±0.5 K (checked in water samples for sample temperatures of 25 °C to 80 °C).

The control algorithm takes into account the defined target temperature of the sample and the measured temperature at the sensors. The measurement can start once the modeled temperature in the sample is achieved with sufficient stability. It is possible that the measurement will begin shortly after the disposable vial has been inserted.

The sample holder identification is used to determine whether the defined sample holder is being used. Sample vessel detection ensures that a sample vessel in the sample holder is utilized. Temperature control ensures that the sample is at the correct temperature for subsequent spectra acquisition.

The temperature sensor is moved away from the sample vessel using the **VESSEL REMOVAL** command if the temperature of the sample has been controlled. This then allows the sample vessel to be removed from the sample holder without damaging the temperature sensor. Temperature control can then be continued in the sample holder or it can also be completely deactivated. As an option, the process sequence can be paused until the sample that has already been analyzed is removed. This allows a controlled run, especially with series determinations.

The temperature control can be switched on with the **PREP SPEC** command and switched off with **VESSEL REMOVAL** command.

Temperature control for the sample holder of the liquid sample presentation can be set manually under **Equipment** ▶ **Instruments** ▶ **Manual control**. Additional information on manual temperature control: *(see "OMNIS NIR Analyzer Liquid – Manual control", chapter 5.12.2.10.2, page 874)*, *(see "OMNIS NIR Analyzer Liquid/Solid – Manual control", chapter 5.12.2.10.4, page 877)*

The maximum duration for temperature control in the spectrometer is 120 minutes. If no measurement with active temperature control is carried out during this time, then temperature control is stopped and the determination is canceled.

See also

OMNIS NIR Analyzer Liquid – Manual control (chapter 5.12.2.10.2, page 874)

OMNIS NIR Analyzer Liquid/Solid – Manual control (chapter 5.12.2.10.4, page 877)

PREP SPEC – Properties (chapter 5.11.8.24.2, page 636)

VESSEL REMOVAL – Properties (chapter 5.11.8.24.1, page 634)

5.11.8.24.1 VESSEL REMOVAL – Properties

The **VESSEL REMOVAL** command is used to safely remove the sample vessel from the sample holder of the liquid sample presentation after the temperature control on the sample vessel has been carried out. To do this, the temperature sensor is moved back from its position and the temperature control at the sample vessel is switched off. In addition, the user can configure whether the command should wait for the sample vessel to be removed and whether temperature control should continue at the sample holder.

The **VESSEL REMOVAL** command must be referenced in the parameters of the **PREP SPEC** command. This is the only way to ensure that the temperature sensor is not damaged when the sample vessel is removed after the temperature control on the sample vessel.

After selecting the **VESSEL REMOVAL** command, double-clicking on the command or clicking on opens the **Properties** window. Additional information on **Create method**: *(see "Creating and editing a method", chapter 5.11.3.3, page 418)*. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the fol-

lowing functions and information are available for the **VESSEL REMOVAL**:

Parameters

Ensure removal of the sample vessel	If the check box is enabled, the user is prompted to remove the sample vessel from the sample holder. The analysis is continued only after the already analyzed sample has been removed and a new sample inserted. The option is disabled by default.
Sample holder temperature control	The temperature control at the sample vessel is switched off for its safe removal. With the additional selection, the user can determine the temperature control on the sample holder: ▪ **Continue** (Default value): The temperature continues to be controlled on the sample holder. **Note**: If no temperature control was previously enabled, then no temperature control will be carried out afterwards. ▪ **Deactivate**: The temperature control on the sample holder is switched off.

The maximum duration for temperature control in the spectrometer is 120 minutes. If no measurement with active temperature control is carried out during this time, then temperature control is stopped and the determination is canceled.

Execute with

In order for a **VESSEL REMOVAL** command to be executed, a functional unit of the **Liquid Sample Presentation** type needs to be assigned to it.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS SPEC – Command variables (chapter 5.11.8.31.1, page 678)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

PREP SPEC – Properties (chapter 5.11.8.24.2, page 636)

Temperature control and sample processing – principle (chapter 5.11.8.24, page 633)

5.11.8.24.2 PREP SPEC – Properties

The **PREP SPEC** command is used for the preparation of spectroscopic analysis of liquid samples using sample holder identification, sample vessel detection and temperature control. The sample holder identification is used to determine whether the defined sample holder is being used. Sample vessel detection ensures that a sample vessel in the sample holder is utilized. Temperature control ensures that the sample is at the correct temperature for subsequent spectra acquisition.

The temperature control in the sample is supported for the following sample vessel types: **Disposable vial 2 mm (67402070), Disposable vial 4 mm (67402250), Disposable vial 8 mm (67402240), Disposable vial 10 mm (67402100)**.

The temperature control in the sample is **not** supported for sample vessels of the **Flow-through cell** and **Cuvette** types. Only the temperature control in the sample holder is available for sample vessels of the **Flow-through cell** and **Cuvette** types.

The temperature control in the sample was validated, based on various criteria:

- Target temperature of the sample: between 25 °C and 80 °C.
- Accuracy ±0.5 K (checked in water samples for sample temperatures of 25 °C to 80 °C).

The control algorithm takes into account the defined target temperature of the sample and the measured temperature at the sensors. The measurement can start once the modeled temperature in the sample is achieved with sufficient stability. It is possible that the measurement will begin shortly after the disposable vial has been inserted.

After selecting the **PREP SPEC** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **PREP SPEC** command:

Parameters

Sample vessel	
Selection of the type	Select the sample vessel that is to be inserted into the sample holder. ▪ **Disposable vial**: If **Disposable vial** is selected, the following specific parameter is displayed: – **Selection of the disposable vial** ▪ **Cuvette**: If **Cuvette** is selected, the following specific parameter is displayed: – **Selection of the cuvette** ▪ **Flow-through cell**: If **Flow-through cell** is selected, the following specific parameter is displayed: – **Selection of the flow-through cell** ▪ **User-specific**: If a sample vessel is used that is not available in the selection list, a user-specific sample vessel can be used. If **User-specific** is selected, the following specific parameter is displayed: – **Name of the sample vessel** **Note**: Sample holder identification is not enabled when a user-specific sample vessel is used.
Selection of the disposable vial	Select the disposable vial that is to be used for the determination. The respective article number is in brackets. The associated sample holder is defined at the same time by selecting the diameter. ▪ **Disposable vial 2 mm (67402070)** ▪ **Disposable vial 4 mm (67402250)** ▪ **Disposable vial 8 mm (67402240)** ▪ **Disposable vial 10 mm (67402100)**
Selection of the cuvette	Select the cuvette that is to be inserted into the sample holder for the determination. The respective article number is in brackets. The associated sample holder is defined at the same time by selecting the optical path length. ▪ **Cuvette 1 mm (67401200)** ▪ **Cuvette 2 mm (67401210)** ▪ **Cuvette 5 mm (67401220)** ▪ **Cuvette 10 mm (67401230)**

Sample vessel	
Selection of the flow-through cell	Select the flow-through cell that is to be inserted for the determination. The respective article number is in brackets. **Note**: All types listed use the same sample holder. This makes it possible to check whether the corresponding sample holder is being used, but not whether the correct type of flow-through cell is being used. ▪ **User-specific flow-through cell**: If a flow-through cell is used that is not available in the selection list, this option can be selected. ▪ **Flow-through cell 0.5 mm (67401300)** ▪ **Flow-through cell 1 mm (67401310)** ▪ **Flow-through cell 2 mm (607401320)** ▪ **Flow-through cell 2.5 mm and 5 mm (607401330)** ▪ **Flow-through cell 5 mm and 10 mm (607401340)**
Name of the sample vessel	If a user-specific sample vessel is used, then a name or a designation for the user-specific sample vessel can be entered in this input field. If the input field is left empty, then **Unspecified sample vessel** will be displayed by default. **Note**: Sample holder identification is not enabled when a user-specific sample vessel is used.

Temperature control	
Setting	Set the temperature control. ▪ **On**: Enable temperature control. ▪ **Off**: Disable temperature control.

Temperature control	
Place of temperature control	Select the place of temperature control. ▪ **Sample holder**: The temperature is controlled directly on the sample holder. ▪ **Sample vessel**: The temperature is controlled directly on the sample vessel **(applicable only for the disposable vials listed above, not applicable for cuvettes or flow-through cells)**. If **Sample vessel** is selected, then the following specific parameter is displayed: – **Command for secure removal of the sample**: Select the **VESSEL REMOVAL** command. If the **VESSEL REMOVAL** command has not yet been added to the method, then add the command to the method no later than at this point and select **Remove sample vessel safely** in the selection list. **Note**: The **VESSEL REMOVAL** command must be executed to ensure that the temperature sensor is not damaged when the sample vessel is removed. **Note**: Alternatively, the sample vessel can be safely removed by **manually** stopping the temperature control of the sample vessel.

Temperature control	
Target temperature	Set the target temperature. The **MEAS SPEC** command triggers spectra acquisition as soon as the set target temperature is reached and remains stable. In this input field, enter the desired target temperature. The entered temperature must be within the permissible range. The default value is **25 °C**. The following input methods are available for selection by clicking on ⌄: ▪ **Formula**: Opens the formula editor in which the calculation formula can be entered or changed: *(see "Formula editor – Brief description", chapter 5.11.9, page 825)*. ▪ **Default value**: Sets the temperature to the default value of 25 °C. ▪ **Enter value**: Enter any target temperature that lies within the specified temperature range.

The maximum duration for temperature control in the spectrometer is 120 minutes. If no measurement with active temperature control is carried out during this time, then temperature control is stopped and the determination is canceled.

Execute with

In order for a **PREP SPEC** command to be executed, a functional unit of the **Liquid Sample Presentation** type needs to be assigned to it.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS SPEC – Command variables (chapter 5.11.8.31.1, page 678)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

Temperature control and sample processing – principle (chapter 5.11.8.24, page 633)

VESSEL REMOVAL – Properties (chapter 5.11.8.24.1, page 634)

5.11.8.25 MEAS COND – Properties

The **MEAS COND** command is used to measure the conductivity of a solution.

The determination can be paused manually during the execution of a **MEAS COND** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

After selecting the **MEAS COND** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS COND** command:

Parameters

Measuring parameters	
Drift-controlled measurement	Selection of the measuring mode. If **Drift-controlled measurement** is selected, the following specific parameters are displayed: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** Drift-controlled measurements are canceled if one of the following criteria is reached: **Signal drift**, **Maximum waiting time** or **Stop measured value**.
Time-controlled measurement	Selection of the measuring mode. If **Time-controlled measurement** is selected, the following specific parameter is displayed: ▪ **Measurement duration** Time-controlled measurements are canceled if one of the following criteria is reached: **Measurement duration** or **Stop measured value**.
Signal drift	The measured value is adopted as soon as the signal drift drops below the defined value.
Minimum waiting time	For drift-controlled measurements, the measured value is not adopted until the minimum waiting time has expired and the measurement has been aborted.
Maximum waiting time	Longest possible waiting time after which the measured value for drift-controlled measurements is adopted and the measurement is aborted, even if the signal drift has not yet been reached or the **Stop measured value** parameter is deactivated.
Measurement duration	For time-controlled measurements, the measurement is aborted as soon as the entered measurement duration is reached.

Measuring parameters	
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the time interval has not yet been reached.
Stop measured value	The measurement is canceled as soon as the specified measured value has been reached. **Off** disables this stop condition.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the measuring solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The manually entered temperature value is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected. This temperature value is saved in the measuring point list and in the command variable '**Temperature.Final**.*Command name*' if the temperature was not measured with a temperature sensor.

Temperature compensation	
Temperature compensation	Selection of the type of temperature compensation. ▪ **Constant factor**: If **Constant factor** is selected, then the following specific parameters appear: – **Reference temperature** – **Temperature coefficient** ▪ **DIN EN 27888**: This type of temperature compensation is used for the determination of ground water, spring water and surface water in accordance with DIN EN 27888. If **DIN EN 27888** is selected, the following specific parameter appears: – **Reference temperature** ▪ **No temperature compensation**
Reference temperature	The electrical conductivity depends greatly on the temperature. The conductivity measured at a particular temperature is automatically converted to the conductivity of this reference temperature (usually 20 °C or 25 °C).
Temperature coefficient	Temperature compensation is carried out with the constant factor entered here.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Conductivity κ** ▪ **Drift** (conductivity difference / time difference) ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Conductivity κ** (default value) ▪ **Drift** (conductivity difference / time difference) ▪ **Temperature**

Chart – y2-axis	
Display y2-axis	Display of a second y-axis for displaying another quantity as a curve.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Conductivity κ** ▪ **Drift** (conductivity difference / time difference) (default value) ▪ **Temperature**

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **MEAS COND** command to be able to be carried out, a functional unit of the **Measuring Module Conductivity** or **Measuring Interface Conductivity** type to which a sensor of the **Conductivity measuring cell** type is connected must be assigned to that command.

After a functional unit for the command has been selected, the following additional parameter appears:

Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS CONC – Properties (chapter 5.11.8.30, page 668)

MEAS COND – Command variables (chapter 5.11.8.25.1, page 644)

MEAS Ipol – Properties (chapter 5.11.8.28, page 657)

MEAS T – Properties (chapter 5.11.8.29, page 663)

MEAS U – Properties (chapter 5.11.8.27, page 651)

MEAS pH – Properties (chapter 5.11.8.26, page 645)

5.11.8.25.1 MEAS COND – Command variables

The following variables are generated by the **MEAS COND** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Driftvalue.Final**.*Command name*' Conductivity drift (end value) after processing the command. This variable is available only for OMNIS instruments. Unit: (mS/cm)/min
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C

Command variables
'**Time.Final**.*Command name*'
Time stamp for the last measuring point in the measuring point list.
Unit: s
'**Unit.Measvalue**.*Command name*'
Unit of the measured values.
Unit: mS/cm

Equipment variables
'**Name.CurrentSensor**.*Command name*'
Name of the sensor used to measure the required measured quantity.

See also

MEAS COND – Properties (chapter 5.11.8.25, page 641)

5.11.8.26 MEAS pH – Properties

The **MEAS pH** command is used to execute potentiometric pH measurements with pH electrodes.

The determination can be paused manually during the execution of a **MEAS pH** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS pH** command:

Parameters

Measuring parameters	
Drift-controlled measurement	Selection of the measuring mode. If **Drift-controlled measurement** is selected, the following specific parameters are displayed: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** Drift-controlled measurements are canceled if one of the following criteria is reached: **Signal drift**, **Maximum waiting time** or **Stop measured value pH**.

Measuring parameters	
Time-controlled measurement	Selection of the measuring mode. If **Time-controlled measurement** is selected, the following specific parameter is displayed: ▪ **Measurement duration** Time-controlled measurements are canceled if one of the following criteria is reached: **Measurement duration** or **Stop measured value pH**.
Signal drift	The measured value is adopted as soon as the signal drift drops below the defined value.
Minimum waiting time	If drift control is activated, the measured value will not be applied until after the minimum waiting time has expired at the earliest, even if the signal drift has already fallen below a defined value.
Maximum waiting time	If drift control is activated, the measured value is adopted no later than after the maximum waiting time has expired, even if the signal drift has not yet been reached or the **Stop measured value pH** parameter is deactivated.
Measurement duration	For time-controlled measurements, the measurement is canceled as soon as the entered measurement duration is reached.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the time interval has not yet been reached.
Stop measured value pH	The measurement is canceled if the stop measured value has been reached since the start of the measurement. The checking of the stop measured value is deactivated with **Off**.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the measuring solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature value that was entered manually under **Temperature** is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously. The temperature value is used to adjust the Nernst slope of the electrode.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected. This temperature value is placed in the measuring point list and in the '**Temperature.Final**.*Command name*' command variable.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **pH** ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **pH** (default value) ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **pH** ▪ **Drift** (potential difference / time difference) (default value) ▪ **Temperature**

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s
- **Stop measured value pH** (Titrando)
  Minimum value: –13.000
  Maximum value: 20.000

- **Stop measured value pH** (855 Robotic Titrosampler)
  Minimum value: –20.000
  Maximum value: 20.000

Execute with

For a **MEAS pH** command to be executed, the corresponding functional unit (and, in the case of analog measuring inputs, the sensor used) must be assigned to it.

- Measuring input (digital or analog):
  Measuring Module Digital, **Measuring Module Analog**, **Measuring Interface iConnect** or **Measuring Interface Analog**.
- Sensor (digital or analog):
  pH electrode

After a functional unit for the command has been selected, the following additional parameters appear:

For **Measuring Module Analog**:	
Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **Difference**: Differential measurement between electrodes at INPUT 1 and INPUT 2.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error. **Note**: For a combined pH/temperature sensor, both measuring inputs must be set to **INPUT 1**.

Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.

For **Measuring Interface Analog** and **Measuring Interface iConnect**:	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **Ind./Ref./Temp.**: Measurement with an analog electrode. ▪ **iConnect**: Measurement with an intelligent electrode (iTrode)
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ► **Parameters** ► **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS CONC – Properties (chapter 5.11.8.30, page 668)

MEAS COND – Properties (chapter 5.11.8.25, page 641)

MEAS Ipol – Properties (chapter 5.11.8.28, page 657)

MEAS T – Properties (chapter 5.11.8.29, page 663)

MEAS U – Properties (chapter 5.11.8.27, page 651)

MEAS pH – Command variables (chapter 5.11.8.26.1, page 650)

5.11.8.26.1 MEAS pH – Command variables

The following variables are generated by the **MEAS pH** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Driftvalue.Final**.*Command name*' Potential drift (end value) after processing the command. Unit: mV/min
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**' variable
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of the measured value.

Equipment variables
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.
'**Slope.CurrentSensor**.*Command name*' Slope of the pH electrode used. Unit: None (standardized to Nernst slope)
'**ZeroPoint.CurrentSensor**.*Command name*' Electrode zero point pH(0) of the pH electrode used. Unit: None

See also

MEAS pH – Properties (chapter 5.11.8.26, page 645)

5.11.8.27 MEAS U – Properties

The **MEAS U** command is used to execute potentiometric voltage measurements.

The determination can be paused manually during the execution of a **MEAS U** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS U** command:

Parameters

Measuring parameters	
Drift-controlled measurement	Selection of the measuring mode. If **Drift-controlled measurement** is selected, the following specific parameters are displayed: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** Drift-controlled measurements are canceled if one of the following criteria is reached: **Signal drift**, **Maximum waiting time** or **Stop measured value**.

Measuring parameters	
Time-controlled measurement	Selection of the measuring mode. If **Time-controlled measurement** is selected, the following specific parameter is displayed: ▪ **Measurement duration** Time-controlled measurements are canceled if one of the following criteria is reached: **Measurement duration** or **Stop measured value**.
Signal drift	The measured value is adopted as soon as the signal drift drops below the defined value.
Minimum waiting time	If drift control is activated, the measured value will not be applied until after the minimum waiting time has expired at the earliest, even if the signal drift has already fallen below a defined value.
Maximum waiting time	If drift control is activated, the measured value is adopted no later than after the maximum waiting time has expired, even if the signal drift has not yet been reached or the **Stop measured value** parameter is deactivated.
Measurement duration	For time-controlled measurements, the measurement is canceled as soon as the entered measurement duration is reached.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the time interval has not yet been reached.
Stop measured value	The measurement is canceled if the stop measured value has been reached since the start of the measurement. The checking of the stop measured value is deactivated with **Off**.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the measuring solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected. This temperature value is placed in the measuring point list and in the '**Temperature.Final**.*Command name*' command variable.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Potential** ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Potential** (default value) ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Potential** ▪ **Drift** (potential difference / time difference) (default value) ▪ **Temperature**

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s
- **Stop measured value** (Titrando)
  Minimum value: –1,200.0 mV
  Maximum value: 1,200.0 mV

- **Stop measured value** (855 Robotic Titrosampler)
  Minimum value: –2,000.0 mV
  Maximum value: 2,000.0 mV

Execute with

For a **MEAS U** command to be executed, the corresponding functional unit (and, in the case of analog measuring inputs, the sensor used) must be assigned to it.

- Measuring input (digital or analog):
  Measuring Module Digital, **Measuring Module Analog**, **Measuring Interface iConnect** or **Measuring Interface Analog**.
- Sensor (digital or analog):
  Ion-selective electrode, **Metal electrode**, **pH electrode** or **Other sensor**

After a functional unit for the command has been selected, the following additional parameters appear:

For **Measuring Module Analog**:	
Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **Difference**: Differential measurement between electrodes at INPUT 1 and INPUT 2.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error. **Note**: For a combined pH/temperature sensor, both measuring inputs must be set to **INPUT 1**.

Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.

For **Measuring Interface Analog** and **Measuring Interface iConnect**:	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **Ind./Ref./Temp.**: Measurement with an analog electrode. ▪ **iConnect**: Measurement with an intelligent electrode (iTrode)
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ► **Parameters** ► **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS CONC – Properties (chapter 5.11.8.30, page 668)

MEAS COND – Properties (chapter 5.11.8.25, page 641)

MEAS Ipol – Properties (chapter 5.11.8.28, page 657)

MEAS T – Properties (chapter 5.11.8.29, page 663)

MEAS U – Command variables (chapter 5.11.8.27.1, page 656)

MEAS pH – Properties (chapter 5.11.8.26, page 645)

5.11.8.27.1 MEAS U – Command variables

The following variables are generated by the **MEAS U** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Driftvalue.Final**.*Command name*' Potential drift (end value) after processing the command. Unit: mV/min
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**' variable
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of the measured value.

Equipment variables
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.
'**Slope.CurrentSensor**.*Command name*' Slope of the pH electrode or ion-selective electrode (ISE) used. Unit: ▪ **pH electrode:** None (standardized to Nernst slope) ▪ **ISE:** mV
'**ZeroPoint.CurrentSensor**.*Command name*' Electrode zero point pH(0) or E(0) of the pH electrode or ion-selective electrode (ISE) used. Unit: ▪ **pH electrode:** None ▪ **ISE:** mV

See also

MEAS U – Properties (chapter 5.11.8.27, page 651)

5.11.8.28 MEAS Ipol – Properties

The **MEAS Ipol** command is used to execute voltametric measurements with a selectable polarization current using polarizable metal electrodes.

The determination can be paused manually during the execution of a **MEAS Ipol** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

After selecting the **MEAS Ipol** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS Ipol** command:

Parameters

Measuring parameters	
Drift-controlled measurement	Selection of the measuring mode. If **Drift-controlled measurement** is selected, the following specific parameters are displayed: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** Drift-controlled measurements are canceled if one of the following criteria is reached: **Signal drift**, **Maximum waiting time** or **Stop measured value**.
Time-controlled measurement	Selection of the measuring mode. If **Time-controlled measurement** is selected, the following specific parameter is displayed: ▪ **Measurement duration** Time-controlled measurements are canceled if one of the following criteria is reached: **Measurement duration** or **Stop measured value**.
Signal drift	The measured value is adopted as soon as the signal drift drops below the defined value.
Minimum waiting time	If drift control is activated, the measured value is always adopted after the minimal waiting time has expired, even if it has already fallen below the **Signal drift**.
Maximum waiting time	Waiting time after which the measured value for drift-controlled measurements is adopted at the latest, even if the signal drift has not yet been reached or the **Stop measured value** parameter is deactivated.
Measurement duration	For time-controlled measurements, the measurement is aborted as soon as the entered measurement duration is reached.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the measuring point time interval has not yet been reached.
Stop measured value	The measurement is canceled if the stop measured value has been reached since the start of the measurement. **Off** deactivates the stop measured value.

Measuring parameters	
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the **Automatic** or **Manual** setting has been selected.
I(pol) DC	The polarization current I(pol) DC (Direct Current) is the current that is applied to the polarizable metal electrode during voltametric measurement. **Note**: For OMNIS instruments, Metrohm recommends entering the current in increments of 0.5 µA. For instruments of the **Titrando** type an increment of 0.5 µA **must** be observed. For instruments of the **855 Robotic Titrosampler** type, an increment of 2.5 µA **must** be observed.
Carry out electrode check	The electrode check is carried out at the beginning of the determination, during the transition from the inactive ground state to the titration. It checks within a few seconds whether an electrode is connected and whether a short circuit is present.
Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Potential** ▪ **Drift** (potential difference / time difference) ▪ **Temperature**
Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Potential** (default value) ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Potential** ▪ **Drift** (potential difference / time difference) (default value) ▪ **Temperature**

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s
- **I(pol) DC** (Titrando)
  Minimum value: –122.5 µA
  Maximum value: 122.5 µA
  Permitted increment: 0.5 µA
- **I(pol) DC** (855 Robotic Titrosampler)
  Minimum value: –122.5 µA
  Maximum value: 122.5 µA
  Permitted increment: 2.5 µA
- **Stop measured value** (Titrando)
  Minimum value: –1,200.0 mV
  Maximum value: 1,200.0 mV
- **Stop measured value** (855 Robotic Titrosampler)
  Minimum value: –2,000.0 mV
  Maximum value: 2,000.0 mV

Execute with

In order for a **MEAS Ipol** command to be executed, the corresponding functional unit must be assigned to it:

Measuring Module Analog, **Measuring Module Coulometry**, **Measuring Interface Analog** or **Interface Coulometry**.

The following parameters must also be defined:

For **Measuring Module Analog** and **Measuring Module Coulometry**:	
Sensor name	Selection of the indicator electrode of the **Polarizable metal electrode** type to be used for the titration. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ► **Parameters** ► **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Measuring Interface Analog**:	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and the functional unit selected: **Pol./Temp.**: Measurement with a polarizable metal electrode and/or a temperature sensor. **Pol.**: Measurement with a polarizable metal electrode.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Temperature sensor	Selection of the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ► **Parameters** ► **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

For **Interface Coulometry**:	
Measuring input	Selection of the analog measuring input. **Ind./Temp.**: Measurement with an analog electrode and/or a temperature sensor.
Sensor name	Selection of the indicator electrode of the **Polarizable metal electrode** type to be used for the titration. If the default value **No sensor** is selected, then the analysis is canceled with an error.

Temperature sensor	Selection of the sensor of the **Temperature sensor** type that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS CONC – Properties (chapter 5.11.8.30, page 668)

MEAS COND – Properties (chapter 5.11.8.25, page 641)

MEAS Ipol – Command variables (chapter 5.11.8.28.1, page 662)

MEAS T – Properties (chapter 5.11.8.29, page 663)

MEAS U – Properties (chapter 5.11.8.27, page 651)

MEAS pH – Properties (chapter 5.11.8.26, page 645)

5.11.8.28.1 MEAS Ipol – Command variables

The following variables are generated by the **MEAS Ipol** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Driftvalue.Final**.*Command name*' Potential drift (end value) after processing the command. Unit: mV/min
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**' variable
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of the measured value.

Equipment variables
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.

See also

MEAS Ipol – Properties (chapter 5.11.8.28, page 657)

5.11.8.29 MEAS T – Properties

The **MEAS T** command is used to execute temperature measurements.

The determination can be paused manually during the execution of a **MEAS T** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

After selecting the **MEAS T** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In

the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS T** command:

Parameters

Measuring parameters	
Drift-controlled measurement	Selection of the measuring mode. If **Drift-controlled measurement** is selected, the following specific parameters are displayed: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** Drift-controlled measurements are canceled if one of the following criteria is reached: **Signal drift**, **Maximum waiting time** or **Stop measured value**.
Time-controlled measurement	Selection of the measuring mode. If **Time-controlled measurement** is selected, the following specific parameter is displayed: ▪ **Measurement duration** Time-controlled measurements are canceled if one of the following criteria is reached: **Measurement duration** or **Stop measured value**.
Signal drift	The measured value is adopted as soon as the signal drift drops below the defined value.
Minimum waiting time	If drift control is enabled, the measured value will not be applied until after the minimum waiting time has expired at the earliest, and the measurement will be aborted, even if it has already fallen below the **Signal drift**.
Maximum waiting time	If drift control is enabled, the measured value is adopted no later than after the maximum waiting time has expired and the measurement will be aborted, even if the signal drift has not yet been reached or the **Stop measured value** parameter is disabled.
Measurement duration	For time-controlled measurements, the measurement is aborted as soon as the entered measurement duration is reached.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the time interval has not yet been reached.
Stop measured value	The measurement is canceled if the stop measured value has been reached since the start of the measurement. The checking of the stop measured value is disabled with **Off**.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Temperature** ▪ **Drift** (temperature difference / time difference)

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Temperature** (default value) ▪ **Drift** (temperature difference / time difference)

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Temperature** ▪ **Drift** (temperature difference / time difference) (default value)

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift**
  Minimum value: 0.1 °C/min
  Maximum value: 999.0 °C/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s

Execute with

In order for a **MEAS T** command to be executed, the corresponding functional unit must be assigned to it:

Measuring Module Digital, **Measuring Module Analog**, **Measuring Module Coulometry**, **Measuring Interface iConnect**, **Measuring Interface Analog** or **Interface Coulometry**

The following parameters must also be defined for all functional units, apart from **Measuring Module Digital**:

For **Measuring Module Analog** and **Measuring Module Coulometry**:	
Sensor name	Selection of the analog sensor that is used at the measuring input: **Ion-selective electrode**, **pH electrode** or **Temperature sensor** If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input	Selection of the analog measuring input. ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.

For **Measuring Interface Analog** and **Measuring Interface iConnect**:	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **Ind./Ref./Temp.**: Measurement with an analog electrode. ▪ **iConnect**: Measurement with an intelligent electrode (iTrode) ▪ **Pol./Temp.**: Measurement with a temperature sensor.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

For **Interface Coulometry**:	
Measuring input	Selection of the analog measuring input. **Ind./Temp.**: Measurement with an analog electrode and/or a temperature sensor.
Sensor name	Selection of the sensor of the **Temperature sensor** type that is to measure the temperature at the measuring input during the analysis. If the default value **No sensor** is selected, then the analysis is canceled with an error.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS CONC – Properties (chapter 5.11.8.30, page 668)

MEAS COND – Properties (chapter 5.11.8.25, page 641)

MEAS Ipol – Properties (chapter 5.11.8.28, page 657)

MEAS T – Command variables (chapter 5.11.8.29.1, page 667)

MEAS U – Properties (chapter 5.11.8.27, page 651)

MEAS pH – Properties (chapter 5.11.8.26, page 645)

5.11.8.29.1 MEAS T – Command variables

The following variables are generated by the **MEAS T** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Driftvalue.Final**.*Command name*' Temperature drift (end value) after processing the command. Unit: °C/min
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**' variable
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s

Command variables
'**Unit.Measvalue**.*Command name*'
Unit of the measured value.

Equipment variables
'**Name.CurrentSensor**.*Command name*'
Name of the sensor used to measure the required measured quantity.

See also

MEAS T – Properties (chapter 5.11.8.29, page 663)

5.11.8.30 MEAS CONC – Properties

The **MEAS CONC** command is used to determine the concentration of an ion by means of direct measurement.

The determination can be paused manually during the execution of a **MEAS CONC** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS CONC** command:

Parameters

Measuring parameters	
Drift-controlled measurement	Selection of the measuring mode. If **Drift-controlled measurement** is selected, the following specific parameters are displayed: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** Drift-controlled measurements are canceled if one of the following criteria is reached: **Signal drift**, **Maximum waiting time** or **Stop measured value**.
Time-controlled measurement	Selection of the measuring mode. If **Time-controlled measurement** is selected, the following specific parameter is displayed: ▪ **Measurement duration** Time-controlled measurements are canceled if one of the following criteria is reached: **Measurement duration** or **Stop measured value**.

Measuring parameters	
Signal drift	The measured value is adopted as soon as the signal drift drops below the defined value.
Minimum waiting time	If drift control is activated, the measured value will not be applied until after the minimum waiting time has expired at the earliest, even if the signal drift has already fallen below a defined value.
Maximum waiting time	Waiting time after which the measured value for drift-controlled measurements is adopted at the latest, even if the signal drift has not yet been reached or the **Stop measured value** parameter is deactivated.
Measurement duration	For time-controlled measurements, the measurement is canceled as soon as the entered measurement duration is reached.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the time interval has not yet been reached.
Stop measured value	The measurement is canceled if the stop measured value has been reached since the start of the measurement. **Off** deactivates the stop measured value.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the measuring solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as measuring temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected. This temperature value is saved in the measuring point list and in the command variable '**Temperature.Final**.*Command name*' if the temperature was not measured with a temperature sensor.
Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Concentration** ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Concentration** (default value) ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Concentration** ▪ **Drift** (potential difference / time difference) (default value) ▪ **Temperature**

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s

Execute with

For a **MEAS CONC** command to be executed, the corresponding functional unit (and, in the case of analog measuring inputs, the sensor used) must be assigned to it.

- Measuring input (digital or analog):
  Measuring Module Digital, **Measuring Module Analog** or **Measuring Interface Analog**.
- Sensor (digital or analog):
  Ion-selective electrode

After a functional unit for the command has been selected, the following additional parameters appear:

For **Measuring Module Analog**:	
Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **Difference**: Differential measurement between electrodes at INPUT 1 and INPUT 2.
Temperature sensor	Selection of the ion-selective electrode or the temperature sensor that is to measure the temperature during the analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties ▶ Parameters ▶ Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.

For **Measuring Interface Analog**:	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: **Ind./Ref./Temp.**: Measurement with an analog electrode.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

Temperature sensor	Selection of the ion-selective electrode or the temperature sensor that is to measure the temperature during the analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS CONC – Command variables (chapter 5.11.8.30.1, page 672)

MEAS COND – Properties (chapter 5.11.8.25, page 641)

MEAS Ipol – Properties (chapter 5.11.8.28, page 657)

MEAS T – Properties (chapter 5.11.8.29, page 663)

MEAS U – Properties (chapter 5.11.8.27, page 651)

MEAS pH – Properties (chapter 5.11.8.26, page 645)

5.11.8.30.1 MEAS CONC – Command variables

The following variables are generated by the **MEAS CONC** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Charge**.*Command name*' Electrical charge of the measured ion.
'**Driftvalue.Final**.*Command name*' Potential drift (end value) after processing the command. Unit: mV/min
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Ion**.*Command name*' Measured ion whose concentration is to be determined with the electrode.
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: Defined in the '**Unit.Measvalue**.*Command name*' variable
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of the measured value.
Equipment variables
'**Blank.CurrentSensor**.*Command name*' Blank value of the calibration standard. Corresponds to the blank value which results from the calibration. If the calibration was carried out with less than 3 calibration standards, the blank value is set to 0. Unit: Defined in the '**Unit.Blank.CurrentSensor**.*Command name*' variable
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.
'**Slope.CurrentSensor**.*Command name*' Slope of the ion-selective electrode (ISE) used. Unit: mV
'**Unit.Blank.CurrentSensor**.*Command name*' Unit of the blank value.

Equipment variables
'**ZeroPoint.CurrentSensor**.*Command name*'
Electrode zero point E(0) of the ion-selective electrode (ISE) used.
Unit: mV

See also

MEAS CONC – Properties (chapter 5.11.8.30, page 668)

5.11.8.31 MEAS SPEC – Properties

The **MEAS SPEC** command is used to acquire a spectrum of a sample. The spectrum represents the absorbance of the sample as a function of the wavelength of the light used.

The **MEAS SPEC** command can be referenced in the parameters of the **PREDICT** command and the **EVAL BASE STATISTICS** command.

After selecting the **MEAS SPEC** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS SPEC** command:

Parameters

Measuring parameters **(only for instruments of the 2060 The NIR type)**	
Channel	Select the measuring channel in which the measured data is recorded.
Window correction	If the check box is activated, a window correction is applied during acquisition of the spectrum. Apply the window correction if the sample is placed on the reactor window. The window correction is activated by default.
Integration time	Select the type of integration time determination. ▪ **Automatic**: The integration time is determined automatically by the instrument. ▪ **Manual**: The integration time is defined manually. If **Manual** is selected, the following specific parameter appears: – **Integration time**
Integration time	A higher integration time improves the signal-to-noise ratio. The signal must not be saturated with an integration time that is too high.

Measuring parameters (only for instruments of the 2060 The NIR type)	
Averaged spectra	Number of spectra that are measured in succession and of which the mean value is to be displayed. A high number of spectra improves the signal-to-noise ratio. The more spectra are measured in succession, the longer the measurement duration.

Measuring parameters (for functional units of the Solid Sample Presentation type)	
Selection of holder	Select the holder to be used for the sample measurement. The respective article number is in brackets. **Note**: To enable optimum focusing, it is very important to select the right holder. ▪ **No holder**: No holder is used for the measurement. The sample is positioned on the glass surface. ▪ **Small holder (607402200)**: The sample vessel is positioned in the small holder OMNIS NIR (60 mm diameter). ▪ **Large holder (607402100)** (Default value) the sample vessel is positioned in the large holder OMNIS NIR (100 mm diameter). ▪ **Flexible holder (607402300)**: The sample is located in a sample vessel, which is positioned with this holder. The holder provides variable adjustment and can be used with different diameters.
Measuring mode	Select the measuring mode that determines the number of measurements. ▪ **Multi-point measurement** (Default value) for heterogeneous solids. The sample is repositioned several times and measured at different positions. The sample is automatically rotated in the holder or manually moved by the user. ▪ **Single-point measurement**: For homogeneous solids. The sample is measured once.
Selection of the sample vessel	Select the sample vessel to be used for the sample measurement. The respective article number is in brackets. Alternatively, a user-specific text or value can also be entered. The following sample vessel types can be selected: ▪ **Disposable vial 15 mm (67402110)** ▪ **Disposable vial 19 mm (67402120)** ▪ **Disposable vial 22 mm (67402130)** ▪ **Disposable vial 28 mm (67402140)** ▪ **Large cup 100 mm (607402110)** ▪ **Petri dish, PS, 100 mm (607402140)** ▪ **Petri dish, Duroplan, 100 mm (607402150)** ▪ **Small cup 60 mm (607402210)** ▪ **Petri dish, PS, 60 mm (607402240)** ▪ **Petri dish, Duroplan, 60 mm (607402250)** ▪ **Transflection vessel 60 mm (607402260)**

Chart – x-axis	
Quantity	Select the specified quantity to be shown in the curve display on the x-axis: ▪ **Wavelength** (default value) ▪ **Absorbance**

Chart – y-axis	
Quantity	Select the specified quantity to be shown in the curve display on the y-axis: ▪ **Wavelength** ▪ **Absorbance** (default value)

Chart – y2-axis	
Display y2-axis	Display of a second y-axis for displaying another quantity as a curve.
Quantity	Select the specified quantity to be shown in the curve display on the second y-axis: ▪ **Wavelength** ▪ **Absorbance** (default value)

Curve simulation **(for instruments of the 2060 The NIR type and functional units of the Liquid Sample Presentation type)**	
Curve selection	Simulated spectra from the selection list can be used to check the determination run. ▪ **None** (Default value) Deactivate the simulation with this selection before analyzing real samples. ▪ **3% water in ethanol (1)** ▪ **3% water in ethanol (2)** ▪ **4% water in ethanol (1)** ▪ **4% water in ethanol (2)** ▪ **5% water in ethanol (1)** ▪ **5% water in ethanol (2)** ▪ **6% water in ethanol (1)** ▪ **6% water in ethanol (2)** ▪ **7% water in ethanol (1)** ▪ **7% water in ethanol (2)** ▪ **8% water in ethanol (1)** ▪ **8% water in ethanol (2)** ▪ **9% water in ethanol (1)** ▪ **9% water in ethanol (2)** ▪ **10% water in ethanol (1)** ▪ **10% water in ethanol (2)** ▪ **11% water in ethanol (1)** ▪ **11% water in ethanol (2)** ▪ **12% water in ethanol (1)** ▪ **12% water in ethanol (2)** ▪ **13% water in ethanol (1)** ▪ **13% water in ethanol (2)** ▪ **14% water in ethanol (1)** ▪ **14% water in ethanol (2)**

Curve simulation **(for functional units of the Solid Sample Presentation type)**	
Curve selection	Simulated spectra from the selection list can be used to check the determination run. ▪ **None** (Default value) Deactivate the simulation with this selection before analyzing real samples. ▪ **Coffee beans**

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **MEAS SPEC** command to be executed, an instrument of the **2060 The NIR** type or a functional unit of the **Liquid Sample Presentation** type or of the **Solid Sample Presentation** type needs to be assigned to the command.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

EVAL BASE STATISTICS – Parameters (chapter 5.11.8.67, page 773)

MEAS REF SPEC – Properties (chapter 5.11.8.20, page 624)

MEAS SPEC – Command variables (chapter 5.11.8.31.1, page 678)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

5.11.8.31.1 MEAS SPEC – Command variables

The following variables are generated by the **MEAS SPEC** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

The following variables are additionally available if a functional unit of the **Liquid Sample Presentation** type was assigned to the command beforehand in **Properties** ▶ **Execute with**.

Table 6

'**TemperatureControlMode.Result**.*Command name*' Place of temperature control ▪ **Inactive**: No temperature control. ▪ **Sample holder**: The temperature was controlled on the sample holder. ▪ **Sample vessel**: The temperature was controlled on the sample vessel.
'**CurrentTemperature.Result**.*Command name*' Current temperature while the command is being executed. Unit: °C

See also

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

5.11.8.32 CAL pH – Properties

The **CAL pH** command is used to calibrate pH electrodes by measuring the potential of solutions with a known pH value. Either pre-defined, commercially available calibration buffers or calibration buffers one creates oneself can be used as calibration buffers. The calibration data for the pH electrode is calculated automatically from the determined measured values.

The determination can be paused manually during the execution of a **CAL pH** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **CAL pH** command:

Parameters

Calibration buffers	
Buffer type	Selection of the buffer type from a list of calibration buffers for pH calibration from various manufacturers. A customized buffer series can also be used as an alternative with **Custom** in the **Equipment** work area under **Custom calibration buffers**.
Number of calibration buffers	Number of calibration buffers necessary for the calibration.

When selecting a commercial buffer series, make sure that the buffer solution used is actually present in the buffer series: *(see "Metrohm buffer type", chapter 5.12.9.2, page 1038), (see "Baker buffer type", chapter 5.12.9.3, page 1039), (see "Beckmann buffer type", chapter 5.12.9.4, page 1040), (see "DIN buffer type (in accordance with DIN standard 19267, 2012)", chapter 5.12.9.5, page 1041), (see "Fisher buffer type", chapter 5.12.9.6, page 1042), (see "Fluka buffer type", chapter 5.12.9.7, page 1043), (see "Hamilton DURACAL buffer type", chapter 5.12.9.8, page 1044), (see "Merck CertiPUR 20/Titrisol buffer type", chapter 5.12.9.9, page 1045), (see "Buffer type Merck CertiPUR 25", chapter 5.12.9.10, page 1046), (see "Mettler Toledo buffer type", chapter 5.12.9.11, page 1046), (see "NIST buffer type", chapter 5.12.9.12, page 1047), (see "Radiometer Analytical buffer type", chapter 5.12.9.13, page 1048)*.

Measuring parameters	
Signal drift	The measured value is adopted as soon as the signal drift drops below the defined value.
Minimum waiting time	The measured value will not be applied until after the minimum waiting time has expired at the earliest, even if the signal drift has already fallen below a defined value.
Maximum waiting time	The measured value is adopted after the maximum waiting time has expired at the latest, even if the signal drift has not yet been reached.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the time interval has not yet been reached.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the calibration buffer can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as calibration temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously. If the temperature is measured with a temperature sensor, then the temperature determined at the first potential measurement will automatically be adopted as the reference temperature. The calibration will be canceled if the temperature recorded during one of the subsequent measurements deviates more than 2 °C from the reference temperature. The temperature value is used to adjust the Nernst slope of the electrode.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected. This temperature value is placed in the measuring point list and in the '**Temperature.Final**.*Command name*' command variable.
Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Potential** ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Potential** (default value) ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Potential** ▪ **Drift** (potential difference / time difference) (default value) ▪ **Temperature**

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s

Execute with

For a **CAL pH** command to be executed, the corresponding functional unit (and, in the case of analog measuring inputs, the sensor used) must be assigned to it.

- Measuring input (digital or analog):
  Measuring Module Digital, **Measuring Module Analog**, **Measuring Interface iConnect**, or **Measuring Interface Analog**.
- Sensor (digital or analog):
  pH electrode

After a functional unit for the command has been selected, the following additional parameters appear:

For **Measuring Module Analog**:	
Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **Difference**: Differential measurement between electrodes at INPUT 1 and INPUT 2.
Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties ► Parameters ► Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error. **Note**: For a combined pH/temperature sensor, both measuring inputs must be set to **INPUT 1**.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.

For **Measuring Interface Analog** and **Measuring Interface iConnect**:	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **Ind./Ref./Temp.**: Measurement with an analog electrode. ▪ **iConnect**: Measurement with an intelligent electrode (iTrode)
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

Temperature sensor	Selection of the pH electrode or the temperature sensor that is to measure the temperature during analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

CAL pH – Calibration principle (chapter 5.11.8.32.1, page 683)

CAL pH – Command variables (chapter 5.11.8.32.2, page 685)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

DET – Properties (chapter 5.11.8.3.1, page 445)

MEAS pH – Properties (chapter 5.11.8.26, page 645)

MET – Properties (chapter 5.11.8.4.1, page 472)

SET – Properties (chapter 5.11.8.6.1, page 512)

5.11.8.32.1 CAL pH – Calibration principle

The slope and the electrode zero point pH(0) are determined at the time of pH calibration. The slope is temperature-dependent and is specified relative to the Nernst slope.

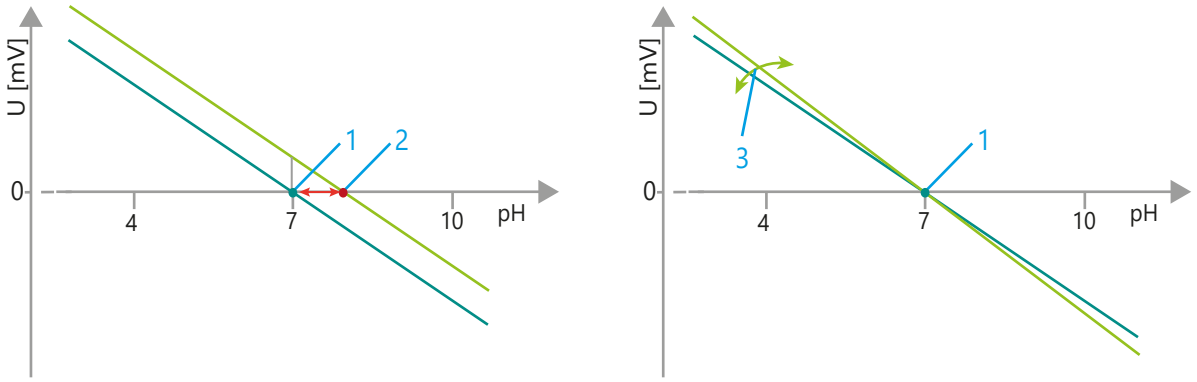


Figure 10 Deviation of the electrode zero point pH(0) and the slope from the ideal Nernst curve.

1 pH(0) of the ideal calibration curve
The zero crossing is at pH 7 and corresponds to a measuring voltage U = 0 mV.

2 pH(0) of a real pH electrode
The zero crossing of a pH electrode is usually not precisely at pH value = 7. This deviation is determined by calibration measurement.

3 Slope of the calibration curve
The slope of the pH electrode is determined via a calibration measurement and specified relative to the Nernst slope.

Relative slope = $S_{measured}/S_{Nernst}$

Buffer solutions with known pH values are used for the pH calibration. Note that the pH value of these buffer solutions is dependent on the temperature. For accurate measurements, the calibration temperature must be the same as the measuring temperature.

The one-point calibration

A buffer solution with known pH value and known temperature is used for the calibration. The theoretical Nernst slope is used as the slope curve of the pH electrode. This corresponds to the relative slope of 1 (100%). The electrode zero point pH(0) is determined by calculation. The calibration data is saved.

The multiple-point calibration

A minimum of 2 different buffer solutions with different pH values are used at a known temperature for the pH calibration. The temperature that is either determined or specified with the first calibration buffer is referred to as the calibration temperature. In the interest of sufficient measuring accuracy, the calibration temperature may not change during the entire calibration. The voltage values for the respective pH values of the calibration buffers are measured at the time of the calibration. The electrode zero point is calculated afterwards via the linear regression of the electrode zero point and the slope (relative to the Nernst slope). After the measurement of the last calibration buffer, the calibration data is saved.

Saving the calibration data

When **digital sensors** are used, the calibration data is written to the memory chip of the pH electrode used. This results in the calibration data being available to all of the systems at which this pH electrode is used.

In the case of **analog sensors**, the calibration data of the pH electrode used is stored in the sensor list. This means that the calibration data is available only to the system with which the calibration was carried out. If the pH electrode is used with other systems, then the calibration must be carried out once more with this pH electrode.

See also

CAL pH – Command variables (chapter 5.11.8.32.2, page 685)

CAL pH – Properties (chapter 5.11.8.32, page 679)

Editing custom calibration buffers (chapter 5.12.9.1.1, page 1036)

5.11.8.32.2 CAL pH – Command variables

The following command variables are generated by the **CAL pH** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Buffervalue.CalibrationSolution**.*Command name*' pH value of the most recently measured calibration buffer. At the time of the calibration, the pH value that was determined is compared to the buffer data of the calibration buffer that is stored in the program. The pH value that is found in the buffer data or interpolated from the temperature is output. Unit: None
'**BuffervaluePrecision**.*Command name*' Number of decimal places of the pH value of the most recently measured calibration buffer. Unit: None
'**CoefficientOfDetermination.Result**.*Command name*' The coefficient of determination R^2 that is output is a quality criterion of linear regression. It indicates how suitable the independent variables are for explaining the variance of the dependent variables. Unit: None
'**Counter.CalibrationSolutions**.*Command name*' Number of the calibration buffers already used during the calibration procedure. Unit: None

'**Driftvalue.Final**.*Command name*'

Potential drift (end value) after processing the command.

Unit: mV/min

'**Duration**.*Command name*'

Total duration for the processing of the command.

Unit: s

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**Measvalue.Final**.*Command name*'

End measured value after processing the command.

Unit: mV

'**Quantity.CalibrationSolutions**.*Command name*'

Number of buffers necessary for the calibration.

Unit: None

'**Slope.Result**.*Command name*'

The relative slope calculated from the calibration in relation to the ideal Nernst slope.

Value range: 0 ... 1 = no match ... exact match

Unit: None

'**Temperature.Final**.*Command name*'

End temperature after processing the command.

Unit: °C

'**Time.Final**.*Command name*'

Time stamp for the last measuring point in the measuring point list.

Unit: s

'**Unit.Measvalue**.*Command name*'

Unit of the measured values.

'**Variance.Result**.*Command name*' Measured value variance of the series. The variance is a measure for the dispersion of the data. Unit: None
'**ZeroPoint.Result**.*Command name*' The electrode zero point of the sensor used calculated from the calibration. Unit: None

Equipment variables
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.

See also

CAL pH – Calibration principle (chapter 5.11.8.32.1, page 683)

CAL pH – Properties (chapter 5.11.8.32, page 679)

5.11.8.33 CAL CONC – Properties

The **CAL CONC** command is used for the calibration of ion-selective electrodes using the potential measurement of solutions with a known ion concentration. The calibration data for the ion-selective electrode is calculated automatically from the determined measured values.

The determination can be paused manually during the execution of a **CAL CONC** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **CAL CONC** command:

Parameters

Calibration standards	
[Define calibration standards]	The subsection for defining the calibration standards is opened. Up to 9 calibration standards can be defined. ▪ **Concentration unit** Selection or entry of the unit for the concentration of the calibration standard. ▪ **Concentration** Entry of the concentration of the calibration standard.

Measuring parameters	
Signal drift	The measured value is adopted as soon as the signal drift drops below the defined value.
Minimum waiting time	The measured value will not be applied until after the minimum waiting time has expired at the earliest, even if the signal drift has already fallen below a defined value.
Maximum waiting time	The measured value is adopted after the maximum waiting time has expired at the latest, even if the signal drift has not yet been reached.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the time interval has not yet been reached.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the calibration standard can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The temperature entered manually under **Temperature** is applied as calibration temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously. If the temperature is measured with a temperature sensor, then the temperature determined at the first potential measurement will automatically be adopted as the reference temperature. The calibration will be canceled if the temperature recorded during one of the subsequent measurements deviates more than 2 °C from the reference temperature.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected. This temperature value is placed in the measuring point list and in the '**Temperature.Final**.*Command name*' command variable.
Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Potential** ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Potential** (default value) ▪ **Drift** (potential difference / time difference) ▪ **Temperature**

Chart – y2-axis	
Display y2-axis	Shows a second y-axis for displaying an additional quantity. The y2-axis is activated via the check box. The display of the y2-axis is deactivated by default.
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Potential** ▪ **Drift** (potential difference / time difference) (default value) ▪ **Temperature**

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

If instruments of the **Titrando** or **855 Robotic Titrosampler** type are used, different input ranges than for OMNIS instruments have to be used for the following parameters:

- **Signal drift**
  Minimum value: 0.1 mV/min
  Maximum value: 999.0 mV/min
- **Time interval measuring point**
  Minimum value: 0.1 s
  Maximum value: 999,999.0 s

Execute with

For a **CAL CONC** command to be executed, the corresponding functional unit (and, in the case of analog measuring inputs, the sensor used) must be assigned to it.

- Measuring input (digital or analog):
  Measuring Module Digital, **Measuring Module Analog** or **Measuring Interface Analog**.
- Sensor (digital or analog):
  Ion-selective electrode

After a functional unit for the command has been selected, the following additional parameters appear:

For **Measuring Module Analog**:	
Sensor name	Selection of the analog sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor. ▪ **Difference**: Differential measurement between electrodes at INPUT 1 and INPUT 2.
Temperature sensor	Selection of the ion-selective electrode or the temperature sensor that is to measure the temperature during the analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties** ▶ **Parameters** ▶ **Titration parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: ▪ **INPUT 1**: Measurement with indicator electrode (with or without combined reference electrode), polarizable electrode or temperature sensor. ▪ **INPUT 2**: Measurement with indicator electrode (with or without combined reference electrode) or temperature sensor.

For **Measuring Interface Analog**:	
Measuring input	Selection of the analog measuring input. The following inputs are available, depending on the command and functional unit selected: **Ind./Ref./Temp.**: Measurement with an analog electrode.
Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

Temperature sensor	Selection of the ion-selective electrode or the temperature sensor that is to measure the temperature during the analysis. If the default value **No temperature sensor** is selected, then the temperature must be entered manually in **Properties ▶ Parameters ▶ Measuring parameters**. If the temperature measuring mode **Continuous** is selected, then the analysis is canceled with an error.

See also

CAL CONC – Calibration principle (chapter 5.11.8.33.1, page 691)

CAL CONC – Command variables (chapter 5.11.8.33.2, page 693)

CAL COND – Properties (chapter 5.11.8.34, page 695)

CAL WRITE – Writing calibration data (chapter 5.11.8.35, page 700)

CAL pH – Properties (chapter 5.11.8.32, page 679)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Ion-selective electrode – Calibrating (chapter 5.12.6.5, page 1010)

MEAS CONC – Properties (chapter 5.11.8.30, page 668)

5.11.8.33.1 CAL CONC – Calibration principle

The **CAL CONC** command is used for the calibration of ion-selective electrodes by means of concentration measurement (direct measurement) of solutions with a known ion concentration. The slope, the zero point and the blank value of the electrode used are calculated from the measured values.

For calibrating ion-selective electrodes (ISE), a linear correlation of the measured potential U_i and the logarithm of the sought ion concentration c_i cannot always be assumed. In ion measurements, interfering ions have an influence on the measurement and that is why this effect is perceptible by a flattening of the curve, especially in low concentration ranges.

The influence of interfering ions can be described by the Nikolsky equation. This is an extended Nernst equation which takes the selectivity of the ion-selective electrode into account. For the calibration with OMNIS, it is used in the following form:

$$U_i = E(0) + \frac{U_{Nernst}}{z} \log(c_i + c_{Blind})$$

The Nernst constant U_{Nernst} represents the theoretical slope S of the calibration function, divided by the charge z of the measuring ion. With anions it has a negative sign, with cations a positive one.

The influence of the interfering ions is indicated as blank value concentration c(blank). A significant blank value reduces the lower measuring range and therefore causes a deterioration of the limit of detection.

For the calibration, there are thus 3 unknown quantities to be calculated for the calibration function, namely the electrode zero point E(0), the slope S and the blank value c(blank). In order to unambiguously calculate all parameters, at least 3 standard measurements are therefore necessary. In order to ensure a higher accuracy of the results, a multiple-point calibration with at least 5 calibration standards is recommended.

Because the ion concentration depends on the temperature, the calibration temperature must not change during the entire calibration for an accurate measurement. The temperature of the standard solution determined at the first measurement will automatically be adopted as the reference temperature. If the temperature of one of the subsequent measurements deviates more than 2 °C from the reference temperature, then the calibration process will automatically be canceled.

In addition, the measured values of the first 2 calibration standards must differ by 6 mV. The difference for the selected unit (ppm, %, mg/L, etc.) must be at least 0.001 between all the defined calibration standards.

The one-point calibration

The calibration is carried out with 1 calibration standard or 1 standard solution with known ion concentration and known temperature. This procedure is only recommended for verifying a solution and is not suitable for carrying out exact measurements.

With the one-point-calibration, only the electrode zero point E(0) is determined by calculation. The theoretical Nernst slope is used for the slope S. The blank value c(blank) is set equal to zero. The calibration data is saved.

The two-point calibration

With the two-point-calibration, the slope for a limited concentration range can be determined by calculation. As long as the ion concentration that needs to be measured is within this range, the two-point-calibration is sufficient.

The calibration is carried out with 2 standard solutions with known ion concentration and known temperature. The slope S and the electrode zero point E(0) are determined by calculation. The blank value c(blank) is set equal to zero. The calibration data is saved.

The three or more point calibration

For accurate measurements, a multiple-point calibration with at least 5 calibration standards is recommended. In order to do so, at least 5 differ-

ent standard solutions with different ion concentrations are used at a known temperature.

Afterwards, the slope S, the electrode zero point E(0) and the blank value c(blank) are calculated iteratively with the Nikolsky evaluation. After the measurement of the last calibration standard, the calibration data is saved.

Saving the calibration data

When **digital sensors** are used, the calibration data is written to the memory chip of the ion-selective electrode used. This results in the calibration data being available to all of the systems at which this ion-selective electrode is used.

In the case of **analog sensors**, the calibration data of the ion-selective electrode used is stored in the sensor list. This means that the calibration data is available only to the system with which the calibration was carried out. If the ion-selective electrode is used with other systems, the calibration data must be transferred manually or the calibration must be carried out once more.

See also

CAL CONC – Command variables (chapter 5.11.8.33.2, page 693)

CAL CONC – Properties (chapter 5.11.8.33, page 687)

Ion-selective electrode – Calibrating (chapter 5.12.6.5, page 1010)

5.11.8.33.2 CAL CONC – Command variables

The following command variables are generated by the **CAL CONC** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Blank.Result**.*Command name*' Blank value of the calibration standard. The variable corresponds to the blank value which results from the calibration. If the calibration was carried out with less than 3 calibration standards, the blank value is set to 0. Unit: Concentration unit of the solution that is added. The unit is defined by the user in the properties of the ion-selective electrode used.
'**CoefficientOfDetermination.Result**.*Command name*' The coefficient of determination R^2 that is output is a quality criterion of linear regression. It indicates how suitable the independent variables are for explaining the variance of the dependent variables. Unit: None

'**Concentration.CalibrationSolution**.*Command name*'

Concentration of the calibration standard that was last measured.

Unit: Concentration unit of the solution that is added. The unit is defined by the user in the properties of the ion-selective electrode used.

'**Counter.CalibrationSolutions**.*Command name*'

Number of the calibration standards already used during the calibration procedure.

Unit: None

'**Driftvalue.Final**.*Command name*'

Potential drift (end value) after processing the command.

Unit: mV/min

'**Duration**.*Command name*'

Total duration for the processing of the command.

Unit: s

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**Measvalue.Final**.*Command name*'

End measured value after processing the command.

Unit: mV

'**Quantity.CalibrationSolutions**.*Command name*'

Number of calibration standards necessary for the calibration.

Unit: None

'**Slope.Result**.*Command name*'

The slope of the electrode calculated from the calibration.

Unit: mV

'**Temperature.Final**.*Command name*'

End temperature after processing the command.

Unit: °C

'**Time.Final**.*Command name*'

Time stamp for the last measuring point in the measuring point list.

Unit: s

'**Unit.Concentration.CalibrationSolution.***Command name*'

Unit of the concentration of the solution that is added. The unit is defined by the user in the properties of the ion-selective electrode used.

'**Unit.Measvalue**.*Command name*'

Unit of the measured values.

'**Variance.Result**.*Command name*'

Measured value variance of the series. The variance is a measure for the dispersion of the data.

Unit: None

'**ZeroPoint.Result**.*Command name*'

The electrode zero point of the sensor used calculated from the calibration.

Unit: mV

Equipment variables

'**Name.CurrentSensor**.*Command name*'

Name of the sensor used to measure the required measured quantity.

See also

CAL CONC – Calibration principle (chapter 5.11.8.33.1, page 691)

CAL CONC – Properties (chapter 5.11.8.33, page 687)

5.11.8.34 CAL COND – Properties

The **CAL COND** command is used for the determination of the cell constant **c** of a conductivity measuring cell.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **CAL COND** command:

Parameters

Conductivity standards	
Definition of standard	Selection of the entry mode of the specifications of the conductivity standard: ▪ **Manual**: The setpoint value of the conductivity standard can be entered manually. If **Manual** is selected, the following parameters are displayed: – **Reference temperature** – **Conductivity κ** – **Temperature coefficient** ▪ **Template**: The setpoint value of the conductivity standard is derived from a template. If **Template** is selected, the template for the standard must be selected with the **Conductivity standard** parameter.
Reference temperature	Temperature at which the conductivity to be measured is known. It should be as close to the measuring temperature as possible.
Conductivity κ	Conductivity κ of the standard at reference temperature.
Temperature coefficient	Temperature coefficient of the standard at reference temperature.
Conductivity standard	Conductivity standards that were defined under **Equipment** ▶ **Solutions** are available in the list.

Measuring parameters	
Drift-controlled measurement	Selection of the measuring mode. If **Drift-controlled measurement** is selected, the following specific parameters are displayed: ▪ **Signal drift** ▪ **Minimum waiting time** ▪ **Maximum waiting time** Drift-controlled measurements are canceled if one of the following criteria is reached: **Signal drift**, **Maximum waiting time** or **Stop measured value**.
Time-controlled measurement	Selection of the measuring mode. If **Time-controlled measurement** is selected, the following specific parameter is displayed: ▪ **Measurement duration** Time-controlled measurements are canceled if one of the following criteria is reached: **Measurement duration** or **Stop measured value**.
Signal drift	The measured value is adopted as soon as the signal drift drops below the defined value.
Minimum waiting time	For drift-controlled measurements, the measured value is not adopted until the minimum waiting time has expired and the measurement has been aborted.

Measuring parameters	
Maximum waiting time	Longest possible waiting time after which the measured value for drift-controlled measurements is adopted and the measurement is aborted, even if the signal drift has not been reached.
Measurement duration	For time-controlled measurements, the measurement is canceled as soon as the entered measurement duration is reached.
Time interval measuring point	Time interval for entering a measuring point into the measuring point list. A measuring point is always entered at the end of the measurement, even if the time interval has not yet been reached.
Temperature measuring mode	Selection of the type of temperature measurement. The temperature of the measuring solution can either be entered manually or measured continuously with a temperature sensor. ▪ **Automatic**: If a temperature sensor is connected, then the temperature will be measured continuously. Otherwise, the temperature entered manually under **Temperature** will be used. ▪ **Manual**: The manually entered temperature value is applied as calibration temperature. ▪ **Continuous**: A temperature sensor must be connected. The temperature is measured continuously.
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected. This temperature value is saved in the measuring point list and in the command variable '**Temperature.Final**.*Command name*' if the temperature was not measured with a temperature sensor.
Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Time** (default value) ▪ **Conductance G** ▪ **Drift** (conductance difference / time difference) ▪ **Temperature**
Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Time** ▪ **Conductance G** (default value) ▪ **Drift** (conductance difference / time difference) ▪ **Temperature**
Chart – y2-axis	
Display y2-axis	Display of a second y-axis for displaying another quantity as a curve.

Chart – y2-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the second y-axis: ▪ **Time** ▪ **Conductance G** ▪ **Drift** (conductance difference / time difference) (default value) ▪ **Temperature**

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **CAL COND** command to be able to be carried out, a functional unit of the **Measuring Module Conductivity** or **Measuring Interface Conductivity** type to which a sensor of the **Conductivity measuring cell** type is connected must be assigned to that command.

After a functional unit for the command has been selected, the following additional parameter appears:

Sensor name	Selection of the sensor that is used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.

See also

CAL CONC – Properties (chapter 5.11.8.33, page 687)

CAL COND – Command variables (chapter 5.11.8.34.1, page 698)

CAL WRITE – Writing calibration data (chapter 5.11.8.35, page 700)

CAL pH – Properties (chapter 5.11.8.32, page 679)

COND CHECK – Parameters (chapter 5.11.8.15, page 606)

Commands – Definition (chapter 5.11.8, page 429)

Creating a Conductivity table (chapter 5.12.10, page 1049)

Creating and editing a method (chapter 5.11.3.3, page 418)

MEAS COND – Properties (chapter 5.11.8.25, page 641)

5.11.8.34.1 CAL COND – Command variables

The following variables are generated by the **CAL COND** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**CellConstant**.*Command name*' Cell constant after processing the command. Unit: cm^{-1}
'**Driftvalue.Final**.*Command name*' Drift for the last measuring point in the measuring point list. Unit: (mS/cm)/min
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Measvalue.Final**.*Command name*' End measured value after processing the command. Unit: mS/cm
'**Temperature.Final**.*Command name*' End temperature after processing the command. Unit: °C
'**Time.Final**.*Command name*' Time stamp for the last measuring point in the measuring point list. Unit: s
'**Unit.Measvalue**.*Command name*' Unit of the measured values. Unit: mS/cm
Equipment variables
'**Name.CurrentSensor**.*Command name*' Name of the sensor used to measure the required measured quantity.

See also

CAL COND – Properties (chapter 5.11.8.34, page 695)

5.11.8.35 CAL WRITE – Writing calibration data

The **CAL WRITE** command is used to backup the calibration data determined in a calibration to the respective sensor. The command can be used to write the calibration data from multiple sensor calibrations onto the respective sensor within an operating procedure. To accomplish this, the command compares the number of measured calibration standards or calibration buffers per sensor used with the number of calibration standards or calibration buffers defined in the respective calibration command.

- When **digital sensors** are used, the calibration data is written to the memory chip of the sensor to be calibrated. This results in the calibration data being available for all of the systems in which this sensor is used.
- With **analog sensors**, the calibration data of the sensor to be calibrated is stored in the local database. This means that the calibration data is available only in the system with which the calibration was carried out. If the sensor is used on different systems, then the calibration data must be transferred manually or this sensor must be recalibrated.

The determination can be paused manually during the execution of a **CAL WRITE** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

The following conditions must be fulfilled in the run in order for the calibration data to be written correctly:

- At least one calibration command (**CAL pH**, **CAL CONC** or **CAL COND**) must have been executed in the method before the **CAL WRITE** command.
- The **CAL WRITE** command must be executed **prior** to the **REPORT** command if a report is to be created in the method. Otherwise the data is not included in the report.

See also

CAL CONC – Properties (chapter 5.11.8.33, page 687)

CAL COND – Properties (chapter 5.11.8.34, page 695)

CAL pH – Properties (chapter 5.11.8.32, page 679)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

5.11.8.36 ADD – Properties

The **ADD** command is used for dosing a solution with a functional unit. The determination can be paused manually during the execution of a **ADD** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

After selecting the **ADD** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **ADD** command:

Parameters

Dosing volume	Volume of solution that is to be added.
Dosing rate	Rate at which the volume increments are dosed. If the dosing rate entered here is higher than the **Maximum dosing rate** defined under **Equipment ▶ Instruments ▶ Specific data ▶ Dosing port ▶** for the inserted functional unit, the latter will be used. In addition, the instrument checks during the execution that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the rate of the functional unit will be reduced. With **Maximum**, the maximum dosing rate defined under **Equipment ▶ Instruments ▶ Specific data ▶ Dosing port ▶ Maximum dosing rate** for the deployed functional unit is used for filling.

Filling rate	Rate at which the cylinder is filled. If the filling rate entered here is higher than the **Maximum filling rate** defined under **Equipment ▶ Instruments ▶ Specific data ▶ Fill port ▶** for the inserted functional unit, then the latter will be used. In addition, the instrument checks during the execution that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the rate of the functional unit will be reduced. With **Maximum**, the maximum filling rate defined under **Equipment ▶ Instruments ▶ Specific data ▶ Fill port ▶ Maximum filling rate** for the inserted functional unit is used to fill.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

For a **ADD** command to be executed, one of the following functional units needs to be assigned to the command:

- **Dosing Drive** with connected **Cylinder Unit**
- **800 Dosino** with connected **807 Dosing Unit**
- **805 Dosimat** with connected **806 Exchange Unit**
- **Internal Dosing Drive** with connected **806 Exchange Unit**

The required solution must be connected to this.

After a functional unit for the command has been selected, the following additional parameters appear:

For **Dosing Drive**:	
Dosing port	Port that is to be used to dose the volume. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1 (default value). ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2.

See also

ADD – Command variables (chapter 5.11.8.36.1, page 703)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

FILL – Properties (chapter 5.11.8.40, page 721)

PISTON END – Properties (chapter 5.11.8.41, page 726)

PISTON POS – Properties (chapter 5.11.8.42, page 731)

5.11.8.36.1 ADD – Command variables

The following variables are generated by the **ADD** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**EndPistonPosition.Result**.*Command name*' Position of the dosing piston in the cylinder unit at which the dosing process was completed. The cylinder length of 50 mm is standardized to a value range of **0** to **1**: ▪ **0** means the dosing piston is at the very bottom. The cylinder is then completely filled. ▪ **1** means the dosing piston is at the very top. The cylinder is then empty. For additional dosing, the cylinder must be filled again. Unit: None (standardized to the total length of the dosing piston)
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**StartPistonPosition.Result**.*Command name*' Position of the dosing piston in the cylinder unit at which the dosing process was started. The cylinder length of 50 mm is standardized to a value range of **0** to **1**: ▪ **0** means the dosing piston is at the very bottom. The cylinder is then completely filled. ▪ **1** means the dosing piston is at the very top. The cylinder is then empty. For additional dosing, the cylinder must be filled again. Unit: None (standardized to the total length of the dosing piston)

Command variables
'**Volume.Final**.*Command name*' End volume after processing the command, i.e. total dosed volume at the end of the command. Unit: mL

Equipment variables
'**Concentration.CurrentSolution**.*Command name*' Concentration of the solution used that is added with the dosing unit or buret (corresponds to the concentration of component 1 in the solution). Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable
'**CylinderVolume.CurrentCylinderUnit**.*Command name*' Cylinder volume of the cylinder unit. Unit: mL
'**Diameter.AspirationTube.CurrentSolution**.*Command name*' Diameter of the aspiration tubing that is connected to the Liquid Adapter. Unit: mm
'**Diameter.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to dosing port 1 of the cylinder unit. Unit: mm
'**Diameter.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to dosing port 2 of the cylinder unit. Unit: mm
'**Diameter.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to the fill port of the cylinder unit. Unit: mm
'**Diameter.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to a special port on the cylinder unit. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the Liquid Adapter. Unit: cm

Equipment variables
'**Length.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 1 of the cylinder unit. Unit: cm
'**Length.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 2 of the cylinder unit. Unit: cm
'**Length.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the fill port of the cylinder unit. Unit: cm
'**Length.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the special port of the cylinder unit. Unit: cm
'**MaxFlowRate.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 1 of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 2 of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for filling at the fill port of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at the special port of the cylinder unit. Unit: mL/min
'**Name.CurrentSolution**.*Command name*' Name of the solution that was added with the dosing unit.
'**SerialNumber.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder unit.
'**SerialNumber.Cylinder.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder.

Equipment variables
'**Titer.CurrentSolution**.*Command name*' Titer of the solution connected to the Liquid Adapter and added using the dosing unit. The titer is the factor that indicates the deviation of the actual concentration from the desired concentration of a titrant. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Unit of the solution's concentration that is added using the dosing unit (corresponds to the unit of concentration for component 1 in the solution). It is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer in the solution connected to the Liquid Adapter that is added using the dosing unit.

See also

ADD – Properties (chapter 5.11.8.36, page 701)

5.11.8.37 ASPIRATE – Properties

The **ASPIRATE** command is used for aspirating a defined volume. The determination can be paused manually during the execution of a **ASPIRATE** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

In the **ASPIRATE** command, the mechanical clearance of the dosing piston is not automatically compensated. If the dosing piston was moved in the opposite direction before (e.g. with an **ADD** or **DOSE** command), a **COMPENSATE** command should be executed as compensation in the method. This ensures high accuracy when pipetting and dosing liquids.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **ASPIRATE** command:

Parameters

Aspiration volume	Volume to be aspirated. If the cylinder is already partly filled, the defined volume must not exceed the remaining cylinder volume, unless the **Enable dispensing** check box is activated.

Aspiration rate	Rate at which the defined volume is to be aspirated. If, in the **Equipment** work area, a **Maximum filling rate** is defined for the selected port of the functional unit used that is smaller than the **Aspiration rate**, then the maximum filling rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are aspirated or if tubing is used that is thinner than standard tubing, then the rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Enable dispensing	If this check box is activated, more volume than the current cylinder volume can be aspirated. To do this, several aspiration steps are executed between which the liquid is dispensed automatically via the selected port. After activation, the following specific parameter is displayed: ▪ **Dispensing rate**
Dispensing rate	Rate at which the liquid is to be dispensed. If, in the **Equipment** work area, a **Maximum dosing rate** is defined for the selected port of the functional unit used that is smaller than the **Dispensing rate**, then the maximum filling rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are aspirated or if tubing is used that is thinner than standard tubing, then the rate needs to be reduced accordingly so that the dosing drive is not overloaded.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

For a **ASPIRATE** command to be executed, one of the following functional units needs to be assigned to the command under **Processes** ▶ **Method** ▶ **Properties** ▶ **Execute with**:

- **Dosing Drive** with connected **Cylinder Unit**
- **800 Dosino** with connected **807 Dosing Unit**

After a functional unit for the command has been selected under **Properties** ▶ **Execute with**, the following additional parameters appear:

For **Dosing Drive**:

Aspiration port	Port via which the liquid is to be aspirated. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening should be moved.
Dispensing port	Port via which the liquid is to be dispensed. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening should be moved.

For **800 Dosino**:	
Aspiration port	Port via which the liquid is to be aspirated. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening should be moved.

See also

ASPIRATE – Command variables (chapter 5.11.8.37.1, page 709)

COMPENSATE – Properties / Execute with (chapter 5.11.8.38, page 712)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

DOSE – Properties (chapter 5.11.8.39, page 716)

5.11.8.37.1 ASPIRATE – Command variables

The following variables are generated by the **ASPIRATE** command during the process sequence and can be used as '**Variable name**.*Command name*' in a formula.

The variables available are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**EndPistonPosition.Result**.*Command name*' Position of the dosing piston in the cylinder at the end of dosing. The stroke of the dosing piston is standardized to a value range of **0** to **1**: ▪ **0** means that the cylinder is completely full. Before aspirating again, the cylinder needs to be emptied. ▪ **1** means that the cylinder is empty. Unit: None (standardized to the stroke of the dosing piston)
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

Command variables

'**StartPistonPosition.Result**.*Command name*'

Position of the dosing piston in the cylinder at the start of dosing. The stroke of the dosing piston is standardized to a value range of **0** to **1**:

- **0** means that the cylinder is completely full. Before aspirating again, the cylinder needs to be emptied.
- **1** means that the cylinder is empty.

Unit: None (standardized to the stroke of the dosing piston)

'**Volume.Final**.*Command name*'

End volume after processing the command, i.e. total aspirated volume at the end of the command.

Unit: mL

Equipment variables

'**Concentration.CurrentSolution**.*Command name*'

Concentration of the solution (e.g. auxiliary solution) that is connected to the cylinder unit or the **807 Dosing Unit**. For solutions of the types **Solution Single-Use** and **Solution Multi-Use**, the concentration of the solution is the same as the concentration of its component 1.

Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable

'**CylinderVolume.CurrentCylinderUnit**.*Command name*'

Volume of the cylinder.

Unit: mL

'**Diameter.AspirationTube.CurrentSolution**.*Command name*'

Diameter of the aspiration tubing that is connected to the cylinder unit or the **807 Dosing Unit**.

Unit: mm

'**Diameter.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*'

Diameter of the connection tubing that is connected to dosing port 1 of the cylinder unit or the **807 Dosing Unit**.

Unit: mm

'**Diameter.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*'

Diameter of the connection tubing that is connected to dosing port 2 of the cylinder unit or the **807 Dosing Unit**.

Unit: mm

Equipment variables
'**Diameter.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to the fill port of the cylinder unit or the **807 Dosing Unit**. Unit: mm
'**Diameter.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to the special port of the cylinder unit or the **807 Dosing Unit**. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the cylinder unit or the **807 Dosing Unit**. Unit: cm
'**Length.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 1 of the cylinder unit or the **807 Dosing Unit**. Unit: cm
'**Length.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 2 of the cylinder unit or the **807 Dosing Unit**. Unit: cm
'**Length.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the fill port of the cylinder unit or the **807 Dosing Unit**. Unit: cm
'**Length.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the special port of the cylinder unit or the **807 Dosing Unit**. Unit: cm
'**MaxFlowRate.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 1 of the cylinder unit or the **807 Dosing Unit**. Unit: mL/min
'**MaxFlowRate.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 2 of the cylinder unit or the **807 Dosing Unit**. Unit: mL/min

Equipment variables
'**MaxFlowRate.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for filling at the fill port of the cylinder unit or the **807 Dosing Unit**. Unit: mL/min
'**MaxFlowRate.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at the special port of the cylinder unit or the **807 Dosing Unit**. Unit: mL/min
'**Name.CurrentSolution**.*Command name*' Name of the solution (e.g. auxiliary solution) that is connected to the cylinder unit or the **807 Dosing Unit**.
'**SerialNumber.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder unit or dosing unit.
'**SerialNumber.Cylinder.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder.
'**Titer.CurrentSolution**.*Command name*' Titer of the solution that is connected to the cylinder unit or the **807 Dosing Unit**. The titer is the factor that indicates the deviation of the actual concentration from the nominal concentration of a titrant. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Unit of the concentration of the solution that is connected to the cylinder unit or the **807 Dosing Unit**. It is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer of the solution that is connected to the cylinder unit or the **807 Dosing Unit**.

See also

ASPIRATE – Properties (chapter 5.11.8.37, page 706)

5.11.8.38 COMPENSATE – Properties / Execute with

The **COMPENSATE** command is used for offsetting the mechanical clearance of the dosing piston, which may occur when changing the direction of the movement. The piston is first moved in the same direction as before and then the piston is moved in the opposite direction.

Metrohm recommends executing a **COMPENSATE** command in the method if the movement direction of the dosing piston has been changed (e.g. with an **ADD** or **DOSE** command). This ensures high accuracy when pipetting and dosing liquids.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. For a **COMPENSATE** command to be executed, one of the following functional units needs to be assigned to the command in the **Execute with** subsection:

- **Dosing Drive** with connected **Cylinder Unit**
- **800 Dosino** with connected **807 Dosing Unit**

After a functional unit for the command has been selected, the following additional parameters appear:

Compensation port	Port via which the mechanical clearance of the dosing piston is to be compensated. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** was selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve opening at the functional unit should be moved.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

ASPIRATE – Properties (chapter 5.11.8.37, page 706)

COMPENSATE – Command variables (chapter 5.11.8.38.1, page 713)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

DOSE – Properties (chapter 5.11.8.39, page 716)

5.11.8.38.1 COMPENSATE – Command variables

The following variables are generated by the **COMPENSATE** command during the process sequence and can be used as '**Variable name**.*Command name*' in a formula.

The variables available are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**Finished**.*Command name*' Status of the command. ▪ **Invalid** means that the command has not been started (yet). ▪ **0** means that the command is still running. ▪ **1** means that the command has been completed correctly. ▪ **2** means that the command has not been completed correctly but that an error or warning occurred. ▪ **3** means that the command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4** means that the command was stopped either with a manual action (by the user: stop or emergency stop), a **STOP** command or because of an error in a command that is running in parallel.

Equipment variables
'**CylinderVolume.CurrentCylinderUnit**.*Command name*' Volume of the cylinder. Unit: mL
'**Diameter.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to dosing port 1 of the functional unit. Unit: mm
'**Diameter.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to dosing port 2 of the functional unit. Unit: mm
'**Diameter.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to the fill port of the functional unit. Unit: mm
'**Diameter.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to the special port of the functional unit. Unit: mm

Equipment variables
'**Length.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 1 of the functional unit. Unit: cm
'**Length.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 2 of the functional unit. Unit: cm
'**Length.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the fill port of the functional unit. Unit: cm
'**Length.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the special port of the functional unit. Unit: cm
'**MaxFlowRate.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 1 of the functional unit. Unit: mL/min
'**MaxFlowRate.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 2 of the functional unit. Unit: mL/min
'**MaxFlowRate.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for filling at the fill port of the functional unit. Unit: mL/min
'**MaxFlowRate.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at the special port of the functional unit. Unit: mL/min
'**SerialNumber.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder unit or dosing unit.
'**SerialNumber.Cylinder.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder.

See also

COMPENSATE – Properties / Execute with (chapter 5.11.8.38, page 712)

5.11.8.39 DOSE – Properties

The **DOSE** command is used for dosing a defined volume. The determination can be paused manually during the execution of a **DOSE** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

In the **DOSE** command, the mechanical clearance of the dosing piston is not automatically compensated. If the dosing piston is to be moved in the opposite direction afterwards (e.g. with an **ASPIRATE** command), a **COMPENSATE** command should be executed as compensation in the method.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **DOSE** command:

Parameters

Dosing volume	Volume to be dosed. If the volume defined here is larger than the remaining cylinder volume, the cylinder unit is filled again automatically via the port that is defined in the command as fill port.
Dosing rate	Rate at which the defined volume is to be dosed. If a smaller **Maximum filling rate** is defined for the selected port of the used functional unit in the **Equipment** work area, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are aspirated or if tubing is used that is thinner than standard tubing, then the rate needs to be reduced accordingly so that the dosing drive is not overloaded.
Filling rate	Rate at which the cylinder is to be filled. If a smaller **Maximum filling rate** is defined for the selected port of the used functional unit in the **Equipment** work area, then this will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are aspirated or if tubing is used that is thinner than standard tubing, then the rate needs to be reduced accordingly so that the dosing drive is not overloaded.

Execute with

In order for a **DOSE** command to be executed, the following functional unit needs to be assigned to the command under **Processes** ▶ **Method** ▶ **Properties** ▶ **Execute with**:

- **Dosing Drive** with connected **Cylinder Unit**
- **800 Dosino** with connected **807 Dosing Unit**

After a functional unit for the command has been selected, the following additional parameters appear:

Dosing port	Port that is to be used to dose the specified volume. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve opening at the functional unit should be moved.
Fill port	Port that is to be used for filling the cylinder. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve opening at the functional unit should be moved.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

COMPENSATE – Properties / Execute with (chapter 5.11.8.38, page 712)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

DOSE – Command variables (chapter 5.11.8.39.1, page 718)

5.11.8.39.1 DOSE – Command variables

The following variables are generated by the **DOSE** command during the process sequence and can be used as '**Variable name**.*Command name*' in a formula.

The variables available are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**Duration**.*Command name*' Total duration for the processing of the command. Unit: s
'**EndPistonPosition.Result**.*Command name*' Position of the dosing piston in the cylinder at the end of dosing. The stroke of the dosing piston is standardized to a value range of **0** to **1**: ▪ **0** means the dosing piston is at the very top. The cylinder is then empty. ▪ **1** means the dosing piston is at the very bottom. The cylinder is then completely filled. Before aspirating again, the cylinder needs to be emptied. Unit: None (standardized to the stroke of the dosing piston)
'**Finished**.*Command name*' Status of the command. ▪ **Invalid** means that the command has not been started (yet). ▪ **0** means that the command is still running. ▪ **1** means that the command has been completed correctly. ▪ **2** means that the command has not been completed correctly but that an error or warning occurred. ▪ **3** means that the command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4** means that the command was stopped either with a manual action (by the user: stop or emergency stop), a **STOP** command or because of an error in a command that is running in parallel.

Command variables

'**StartPistonPosition.Result**.*Command name*'

Position of the dosing piston in the cylinder at the start of dosing. The stroke of the dosing piston is standardized to a value range of **0** to **1**:

- **0** means the dosing piston is at the very bottom. The cylinder is then completely filled. Before aspirating again, the cylinder needs to be emptied.
- **1** means the dosing piston is at the very top. The cylinder is then empty.

Unit: None (standardized to the stroke of the dosing piston)

'**Volume.Final**.*Command name*'

End volume after processing the command, i.e. total dosed volume at the end of the command.

Unit: mL

Equipment variables

'**Concentration.CurrentSolution**.*Command name*'

Concentration of the solution (e.g. auxiliary solution) that is connected to the dosing unit (corresponds to the concentration of component 1 in the solution).

Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable

'**CylinderVolume.CurrentCylinderUnit**.*Command name*'

Volume of the cylinder.

Unit: mL

'**Diameter.AspirationTube.CurrentSolution**.*Command name*'

Diameter of the aspiration tubing that is connected to the functional unit.

Unit: mm

'**Diameter.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*'

Diameter of the connection tubing that is connected to dosing port 1 of the functional unit.

Unit: mm

'**Diameter.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*'

Diameter of the connection tubing that is connected to dosing port 2 of the functional unit.

Unit: mm

'**Diameter.Tube.FillPort.CurrentCylinderUnit**.*Command name*'

Diameter of the connection tubing that is connected to the fill port of the functional unit.

Unit: mm

Equipment variables
'**Diameter.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to the special port of the functional unit. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the functional unit. Unit: cm
'**Length.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 1 of the functional unit. Unit: cm
'**Length.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 2 of the functional unit. Unit: cm
'**Length.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the fill port of the functional unit. Unit: cm
'**Length.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the special port of the functional unit. Unit: cm
'**MaxFlowRate.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 1 of the functional unit. Unit: mL/min
'**MaxFlowRate.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 2 of the functional unit. Unit: mL/min
'**MaxFlowRate.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for filling at the fill port of the functional unit. Unit: mL/min
'**MaxFlowRate.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at the special port of the functional unit. Unit: mL/min

Equipment variables
'**Name.CurrentSolution**.*Command name*' Name of the solution (e.g. auxiliary solution) that is connected to the dosing device.
'**SerialNumber.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder unit or dosing unit.
'**SerialNumber.Cylinder.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder.
'**Titer.CurrentSolution**.*Command name*' Titer of the solution that is connected to the functional unit. The titer is the factor that indicates the deviation of the actual concentration from the desired concentration of a titrant. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Unit of the concentration of the solution that is connected to the dosing device (corresponds to the unit of the concentration of component 1 in the solution). It is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer of the solution that is connected to the dosing device.

See also

DOSE – Properties (chapter 5.11.8.39, page 716)

5.11.8.40 FILL – Properties

The **FILL** command is used for filling the cylinder with the solution connected to the functional unit. The determination can be paused manually during the execution of a **FILL** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

Clicking on under **Processes** ► **Method** ► **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **FILL** command:

Parameters

Fill level	Volume to which the cylinder is filled. If the cylinder is already partly filled, then only the difference in volume will be filled. If an **MSB dosing device** is connected, then the volume entered is ignored and it is automatically filled to **Maximum**. With **Maximum**, it will be filled up to the maximum possible fill level of the cylinder unit used.
Filling rate	Rate at which filling takes place. If the filling rate entered here is higher than the **Maximum filling rate** defined under **Equipment** ▶ **Instruments** ▶ **Specific data** ▶ **Fill port** ▶ for the inserted functional unit, the latter will be used. In addition, the instrument checks during the execution that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the rate of the functional unit will be reduced. With **Maximum**, the maximum filling rate defined under **Equipment** ▶ **Instruments** ▶ **Specific data** ▶ **Fill port** ▶ **Maximum filling rate** for the inserted functional unit is used to fill.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

For a **FILL** command to be executed, one of the following functional units needs to be assigned to the command:

- **Dosing Drive** with connected **Cylinder Unit**
- **800 Dosino** with connected **807 Dosing Unit**
- **805 Dosimat** with connected **806 Exchange Unit**
- **Internal Dosing Drive** with connected **806 Exchange Unit**

The required solution must be connected to this.

After a functional unit for the command has been selected, the following additional parameter appears:

Port	Port via which the cylinder is to be filled. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Current port**: Port that is active at the time the command is executed. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**

See also

805 Dosimat – Properties (chapter 5.12.3.6, page 907)

ADD – Properties (chapter 5.11.8.36, page 701)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Dosing device (MSB) – Properties (chapter 5.12.3.7, page 909)

Dosing unit (OMNIS) – Properties (chapter 5.12.3.8, page 913)

FILL – Command variables (chapter 5.11.8.40.1, page 723)

PISTON END – Properties (chapter 5.11.8.41, page 726)

PISTON POS – Properties (chapter 5.11.8.42, page 731)

5.11.8.40.1 FILL – Command variables

The following variables are generated by the **FILL** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**EndPistonPosition.Result**.*Command name*' Position of the dosing piston in the cylinder unit at which the filling procedure was completed. The cylinder length of 50 mm is standardized to a value range of **0** to **1**: ▪ **0** means the dosing piston is at the very bottom. The cylinder is then completely filled. ▪ **1** means the dosing piston is at the very top. The cylinder is then empty. For additional dosing, the cylinder must be filled again. Unit: None (standardized to the total length of the dosing piston)

Command variables

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**StartPistonPosition.Result**.*Command name*'

Position of the dosing piston in the cylinder unit at which the filling procedure was started. The cylinder length of 50 mm is standardized to a value range of **0** to **1**:

- **0** means the dosing piston is at the very bottom. The cylinder is then completely filled.
- **1** means the dosing piston is at the very top. The cylinder is then empty. For additional dosing, the cylinder must be filled again.

Unit: None (standardized to the total length of the dosing piston)

Equipment variables

'**Concentration.CurrentSolution**.*Command name*'

Concentration of the solution that is used to fill the cylinder (corresponds to the concentration of component 1 in the solution).

Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable

'**CylinderVolume.CurrentCylinderUnit**.*Command name*'

Cylinder volume of the cylinder unit.

Unit: mL

'**Diameter.AspirationTube.CurrentSolution**.*Command name*'

Diameter of the aspiration tubing that is connected to the Liquid Adapter.

Unit: mm

'**Diameter.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*'

Diameter of the connection tubing that is connected to dosing port 1 of the cylinder unit.

Unit: mm

'**Diameter.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*'

Diameter of the connection tubing that is connected to dosing port 2 of the cylinder unit.

Unit: mm

Equipment variables
'**Diameter.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to the fill port of the cylinder unit. Unit: mm
'**Diameter.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to a special port on the cylinder unit. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the Liquid Adapter. Unit: cm
'**Length.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 1 of the cylinder unit. Unit: cm
'**Length.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 2 of the cylinder unit. Unit: cm
'**Length.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the fill port of the cylinder unit. Unit: cm
'**Length.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the special port of the cylinder unit. Unit: cm
'**MaxFlowRate.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 1 of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 2 of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for filling at the fill port of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at the special port of the cylinder unit. Unit: mL/min

Equipment variables
'**Name.CurrentSolution**.*Command name*' Name of the solution used with the dosing unit.
'**SerialNumber.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder unit.
'**SerialNumber.Cylinder.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder.
'**Titer.CurrentSolution**.*Command name*' Titer of the solution connected to the Liquid Adapter and used for filling the cylinder. The titer is the factor that indicates the deviation of the actual concentration from the desired concentration of a titrant. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Unit of the concentration of the solution used for filling the cylinder (corresponds to the unit of concentration for component 1 in the solution). It is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer in the solution connected to the Liquid Adapter and used for filling the cylinder.

See also

FILL – Properties (chapter 5.11.8.40, page 721)

5.11.8.41 PISTON END – Properties

The **PISTON END** command is used to empty the cylinder completely. To do so, the piston in the cylinder is moved downwards until it stops. The determination can be paused manually during the execution of a **PISTON END** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or canceled over the status menu.

The **PISTON END** command for emptying the cylinder completely may only be used for rinsing processes and for cleaning processes.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **PISTON END** command:

Parameters

Flow rate	Enter the rate at which the liquid is dispensed from the cylinder unit. The defined flow rate is used up to position 1. A reduced rate is then used to the end. The flow rate must be reduced accordingly if viscous solutions are used or thinner tubing than the standard tubing is used.

The maximum dosing and filling rates that were defined in the Equipment are not taken into consideration for this command.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

For a **PISTON END** command to be executed, one of the following functional units needs to be assigned to the command:

- **Dosing Drive** with connected **Cylinder Unit**
- **800 Dosino** with connected **807 Dosing Unit**

After a functional unit for the command has been selected, the following additional parameter appears:

Port	Port that is to be used for emptying the cylinder. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Current port**: Port where the valve disk opening is positioned at the time the command is executed. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**

See also

ADD – Properties (chapter 5.11.8.36, page 701)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

FILL – Properties (chapter 5.11.8.40, page 721)

PISTON END – Command variables (chapter 5.11.8.41.1, page 728)

PISTON POS – Properties (chapter 5.11.8.42, page 731)

5.11.8.41.1 PISTON END – Command variables

The following variables are generated by the **PISTON END** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**EndPistonPosition.Result**.*Command name*' Position of the dosing piston in the cylinder unit at which the command was completed. The cylinder length of 50 mm is standardized to a value range of **0** to **1**: ▪ **0** means the dosing piston is at the very bottom. The cylinder is then completely filled. ▪ **1** means the dosing piston is at the very top. The cylinder is then empty. For additional dosing, the cylinder must be filled again. Unit: none (standardized to the total length of the dosing piston)
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**StartPistonPosition.Result**.*Command name*' Position of the dosing piston in the cylinder unit at which the command was started. The cylinder length of 50 mm is standardized to a value range of **0** to **1**: ▪ **0** means the dosing piston is at the very bottom. The cylinder is then completely filled. ▪ **1** means the dosing piston is at the very top. The cylinder is then empty. For additional dosing, the cylinder must be filled again. Unit: none (standardized to the total length of the dosing piston)

Equipment variables
'**Concentration.CurrentSolution**.*Command name*' Concentration of the solution connected to the Liquid Adapter that is added using the dosing unit (corresponds to the concentration of component 1 in the solution). Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable

Equipment variables
'**CylinderVolume.CurrentCylinderUnit**.*Command name*' Cylinder volume of the cylinder unit. Unit: mL
'**Diameter.AspirationTube.CurrentSolution**.*Command name*' Diameter of the aspiration tubing that is connected to the Liquid Adapter. Unit: mm
'**Diameter.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to dosing port 1 of the cylinder unit. Unit: mm
'**Diameter.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to dosing port 2 of the cylinder unit. Unit: mm
'**Diameter.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to the fill port of the cylinder unit. Unit: mm
'**Diameter.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to a special port on the cylinder unit. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the Liquid Adapter. Unit: cm
'**Length.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 1 of the cylinder unit. Unit: cm
'**Length.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 2 of the cylinder unit. Unit: cm
'**Length.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the fill port of the cylinder unit. Unit: cm

Equipment variables
'**Length.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the special port of the cylinder unit. Unit: cm
'**MaxFlowRate.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 1 of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 2 of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for filling at the fill port of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at the special port of the cylinder unit. Unit: mL/min
'**Name.CurrentSolution**.*Command name*' Name of the solution used with the dosing unit.
'**SerialNumber.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder unit.
'**SerialNumber.Cylinder.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder.
'**Titer.CurrentSolution**.*Command name*' Titer of the solution connected to the Liquid Adapter and added using the dosing unit. The titer is the factor that indicates the deviation of the actual concentration from the desired concentration of a standard solution. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Unit of the solution's concentration that is added using the dosing unit (corresponds to the unit of concentration for component 1 in the solution). It is defined by the user in the properties of the solution.
'**Unit.Titer.CurrentSolution**.*Command name*' Unit of the titer in the solution connected to the Liquid Adapter that is added using the dosing unit.

See also

PISTON END – Properties (chapter 5.11.8.41, page 726)

5.11.8.42 PISTON POS – Properties

The **PISTON POS** command is used to move the piston to a certain position in the cylinder, regardless of the current piston position. The determination can be paused manually during the execution of a **PISTON POS** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or canceled over the status menu.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **PISTON POS** command:

Parameters

Target position	Enter the position to which the piston is moved. The positions depend on the functional unit. Functional unit of the type **Dosing Drive**: ▪ Position **1.00000**: The piston is located at the top end of the cylinder's working area. ▪ Position **0.00000**: The piston is located at the bottom end of the cylinder's working area. Functional unit of the type **800 Dosino**: ▪ Position **0.00000**: The piston is located at the top end of the cylinder's working area. ▪ Position **1.00000**: The piston is located at the bottom end of the cylinder's working area.
Flow rate	Enter the rate at which the piston is moved to the target position. The flow rate must be reduced accordingly if viscous solutions are used or thinner tubing than the standard tubing is used.

The maximum dosing and filling rates that were defined in the Equipment are not taken into consideration for this command.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

For a **PISTON POS** command to be executed, one of the following functional units needs to be assigned to the command:

- **Dosing Drive** with connected **Cylinder Unit**
- **800 Dosino** with connected **807 Dosing Unit**

See also

ADD – Properties (chapter 5.11.8.36, page 701)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

FILL – Properties (chapter 5.11.8.40, page 721)

PISTON END – Properties (chapter 5.11.8.41, page 726)

PISTON POS – Command variables (chapter 5.11.8.42.1, page 732)

5.11.8.42.1 PISTON POS – Command variables

The following variables are generated by the **PISTON POS** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The available variables are stored in the **Command variables** and **Equipment variables** variable categories.

Command variables
'**EndPistonPosition.Result**.*Command name*' Position of the dosing piston in the cylinder unit at which the dosing process was completed. The cylinder length of 50 mm is standardized to a value range of **0** to **1**: ▪ **0** means the dosing piston is at the very bottom. The cylinder is then completely filled. ▪ **1** means the dosing piston is at the very top. The cylinder is then empty. For additional dosing, the cylinder must be filled again. Unit: none (standardized to the total length of the dosing piston)
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**StartPistonPosition.Result**.*Command name*' Position of the dosing piston in the cylinder unit at which the dosing process was started. The cylinder length of 50 mm is standardized to a value range of **0** to **1**: ▪ **0** means the dosing piston is at the very bottom. The cylinder is then completely filled. ▪ **1** means the dosing piston is at the very top. The cylinder is then empty. For additional dosing, the cylinder must be filled again. Unit: none (standardized to the total length of the dosing piston)

Equipment variables
'**Concentration.CurrentSolution**.*Command name*' Concentration of the solution connected to the Liquid Adapter that is added using the dosing unit (corresponds to the concentration of component 1 in the solution). Unit: Defined in the 'Unit.Concentration.CurrentSolution' variable
'**CylinderVolume.CurrentCylinderUnit**.*Command name*' Cylinder volume of the cylinder unit. Unit: mL
'**Diameter.AspirationTube.CurrentSolution**.*Command name*' Diameter of the aspiration tubing that is connected to the Liquid Adapter. Unit: mm
'**Diameter.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to dosing port 1 of the cylinder unit. Unit: mm
'**Diameter.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to dosing port 2 of the cylinder unit. Unit: mm
'**Diameter.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to the fill port of the cylinder unit. Unit: mm
'**Diameter.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Diameter of the connection tubing that is connected to a special port on the cylinder unit. Unit: mm
'**Length.AspirationTube.CurrentSolution**.*Command name*' Length of the aspiration tubing that is connected to the Liquid Adapter. Unit: cm
'**Length.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 1 of the cylinder unit. Unit: cm
'**Length.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to dosing port 2 of the cylinder unit. Unit: cm

Equipment variables
'**Length.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the fill port of the cylinder unit. Unit: cm
'**Length.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the special port of the cylinder unit. Unit: cm
'**MaxFlowRate.Tube.DosingPort1.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 1 of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.DosingPort2.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at dosing port 2 of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.FillPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for filling at the fill port of the cylinder unit. Unit: mL/min
'**MaxFlowRate.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Maximum permissible flow rate for dosing at the special port of the cylinder unit. Unit: mL/min
'**Name.CurrentSolution**.*Command name*' Name of the solution used with the dosing unit.
'**SerialNumber.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder unit.
'**SerialNumber.Cylinder.CurrentCylinderUnit**.*Command name*' Serial number of the cylinder.
'**Titer.CurrentSolution**.*Command name*' Titer of the solution connected to the Liquid Adapter and added using the dosing unit. The titer is the factor that indicates the deviation of the actual concentration from the desired concentration of a standard solution. Unit: Defined in the '**Unit.Titer.CurrentSolution**' variable
'**Unit.Concentration.CurrentSolution**.*Command name*' Unit of the solution's concentration that is added using the dosing unit (corresponds to the unit of concentration for component 1 in the solution). It is defined by the user in the properties of the solution.

Equipment variables
'**Unit.Titer.CurrentSolution**.*Command name*'
Unit of the titer in the solution connected to the Liquid Adapter that is added using the dosing unit.

See also

PISTON POS – Properties (chapter 5.11.8.42, page 731)

5.11.8.43 SOLVENT HANDLING – Properties

The **SOLVENT HANDLING** command is used for conveying liquids with the OMNIS Solvent Module.

If a key on the OMNIS Solvent Module is pressed when processing the **SOLVENT HANDLING** command, the command and the pumping are ended.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **SOLVENT HANDLING** command:

Parameters

Function	▪ **Add**: The liquid is conveyed out of the bottle (e.g. from a supply bottle to a titration cell). ▪ **Aspirate**: The liquid is aspirated into to bottle (e.g. from a titration cell to a waste bottle).
Pumping duration	Duration during which liquid is conveyed.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **SOLVENT HANDLING** command to be executed, a functional unit of the **OMNIS Solvent Module** type needs to be assigned to the command.

See also

ADD – Properties (chapter 5.11.8.36, page 701)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

FILL – Properties (chapter 5.11.8.40, page 721)

5.11.8.44 VALVE POS – Properties

The **VALVE POS** command is used for switching the port on the dosing unit. The determination can be paused manually during the execution of a **VALVE POS** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. The **VALVE POS** command will be executed until the end and the determination of the subsample is subsequently held. A held subsample can be continued or canceled over the status menu.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **VALVE POS** command:

Parameters

Target position	Select the port towards which the valve opening on the dosing unit is moved: ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve opening at the functional unit is moved.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

For a **VALVE POS** command to be executed, one of the following functional units needs to be assigned to the command:

- **Dosing Drive** with connected **Cylinder Unit**
- **800 Dosino** with connected **807 Dosing Unit**

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

PISTON END – Properties (chapter 5.11.8.41, page 726)

PISTON POS – Properties (chapter 5.11.8.42, page 731)

5.11.8.45 OPEN GRIPPER – Properties

The **OPEN GRIPPER** command is used for opening the gripper fingers on the gripper arm of the sample robot. Once the gripper is over the sample vessel to be moved, the vessel measurements must be read out. For sample beakers, the opening radius of the gripper fingers is determined automatically by the diameter of the sample beaker to be moved. For vials, the opening radius is automatically determined by the diameter of the vial cap.

After selecting the **OPEN GRIPPER** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In order for a **OPEN GRIPPER** command to be executed, a functional unit of the **Main Module Pick&Place** or **OMNIS Main Module** type needs to have been assigned to it beforehand in the **Execute with** subsection.

See also

CLOSE GRIPPER – Properties (chapter 5.11.8.46, page 737)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

MOVE TO RACK – Properties (chapter 5.11.8.50, page 744)

5.11.8.46 CLOSE GRIPPER – Properties

The **CLOSE GRIPPER** command is used to close the gripper fingers on the gripper arm of the sample robot around the sample vessel so that it can be moved with a secure grip.

After selecting the **CLOSE GRIPPER** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In order for a **CLOSE GRIPPER** command to be executed, a functional unit of the **Main Module Pick&Place** or **OMNIS Main Module** type needs to have been assigned to it beforehand in the **Execute with** subsection.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

OPEN GRIPPER – Properties (chapter 5.11.8.45, page 737)

5.11.8.47 INIT MAIN MODULE – Properties / Execute with

The **INIT MAIN MODULE** command is used to initialize the sample rack that is attached to the turntable of the **sample changer**. This means that the attached rack and the lift are reset, the rack name is read out and the respective rack data is transferred to the sample changer.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In order for an **INIT MAIN MODULE** command to be executed, a functional unit of the **Tower** type needs to have been assigned to it beforehand in the **Execute with** subsection.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

5.11.8.48 LIFT – Properties

The **LIFT** command is used to move the lifts of sample robots or sample changers to a defined lift height.

After selecting the **LIFT** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available, depending on the assigned functional unit for the **LIFT** command:

Parameters

Target height

Select a defined height to which the lift is moved. Depending on the functional unit used, the following parameters are displayed:

Main Module Pick&Place and OMNIS Main Module

- **Enter height**: Entry of an absolute height to which the lift is moved. If **Enter height** is selected, then the following specific parameter appears:
  - **Lift height**

Note: The substitute values **Work height**, **Rinse height**, **Change height** and **Special height** are displayed in the selection list. However, they are not used by the **Main Module Pick&Place** and **OMNIS Main Module** functional units.

Oven Module

- **Work height**: Lift height at which the main task is to be executed at the corresponding turntable position: The vial transfer at the handover position, the start of the analysis at the analysis position, and the conditioning of the system at the conditioning position. The work height for each turntable position can be defined in the specific data.
- **Change height**: Lift height that enables collision-free transport between handover position and analysis position. If there is no vial in the vial holder, it must also be possible to move to and leave the conditioning tube without collision at this height. The change height for each turntable position can be defined in the specific data.
- **Special height**: Lift height at the analysis position of the turntable at which the vial can be transferred from the vial cradle to the vial holder or vice versa. This special height can be defined in the specific data. It is defined by the work height of the handover position.
- **Enter height**: Entry of an absolute height to which the lift is to be moved. If **Enter height** is selected, then the following specific parameter appears:
  - **Lift height**

Tower

- **Work height**: Height that is defined for positions on the rack in the properties of the sample rack and for external positions in the properties of the **786 Swing Head** as the work height. A separate work height can be defined for each special position and each external position.
- **Rinse height**: Height that is defined for positions on the rack in the properties of the sample rack and for external positions in the properties of the **786 Swing Head** as rinse height.
- **Change height**: Height that is defined for positions on the rack in the properties of the sample rack as change height.
- **Special height**: Height that is defined for positions on the rack in the properties of the sample rack as special height.
- **Enter height**: Entry of an absolute height to which the lift is moved. If **Enter height** is selected, then the following specific parameter appears:
  - **Lift height**

Note: The substitute values **Work height**, **Rinse height**, **Change height** and **Special height** can only be used with instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**.

Note: If substitute values are selected, the lift uses the specific lift height that is defined for the position in which the lift is when the command is executed. Additional information on defining lift heights: *(see "Defining the lift height", chapter 5.12.3.30.3, page 978)*.

Lift height	Enter the height (in mm) to which the lift is to be moved. A lift height of **0 mm** corresponds to the home position: The lift is moved all the way to the top. **Note**: If, in the **Equipment** work area, a **Maximum lift height** is entered for the functional unit used that is smaller than the **Lift height** defined here, then an error message will be displayed. In addition, the instrument checks during dosing that this height does not exceed the maximum permitted height for the functional unit used.
Lift rate	Enter the speed (in mm/s) at which the lift is to be moved. The default value **Maximum** corresponds to the maximum speed that is permitted by the functional unit used. **Note**: When execution is carried out on the instrument, a check is made to ensure that this speed does not exceed the maximum permitted speed of the functional unit used. An error message is displayed if the value defined here exceeds the maximum permitted lift rate.

Additional information on the parameters (e.g., input range, unit, default value) can be found in the tooltips.

Parameters with different input ranges

Depending on the functional unit or instrument used, different input ranges apply for the following parameters:

- **Lift height**
  - **Main Module Pick&Place**:
    Minimum value: 0 mm
    Maximum value: 202.0 mm
  - **OMNIS Main Module**:
    Minimum value: 0 mm
    Maximum value: 202.0 mm
  - **Oven Module**:
    Minimum value: 0 mm
    Maximum value: 193.0 mm
  - **Pick&Place Module**:
    Minimum value: 0 mm
    Maximum value: 130.0 mm
  - **Tower** (**814 USB Sample Processor**):
    Minimum value: 0 mm
    Maximum value: 235.0 mm
  - **Tower** (**815 Robotic USB Sample Processor XL**):
    Minimum value: 0 mm
    Maximum value: 235.0 mm
  - **Tower** (**855 Robotic Titrosampler**):
    Minimum value: 0 mm
    Maximum value: 235.0 mm
  - **Tower** (**874 Oven Sample Processor**):
    Minimum value: 0 mm
    Maximum value: 155.0 mm
- **Lift rate**
  - **Main Module Pick&Place** or **OMNIS Main Module** and **Pick&Place Module**:
    Minimum value: 1 mm/s
    Maximum value: 75 mm/s
  - **Oven Module**:
    Minimum value: 10 mm/s
    Maximum value: 100 mm/s
  - **Tower** (all sample changers):
    Minimum value: 5 mm/s
    Maximum value: 25 mm/s

Execute with

For a **LIFT** command to be executed, one of the following functional units needs to be assigned to the command:

- **Main Module Pick&Place**
- **OMNIS Main Module**
- **Oven Module**
- **Pick&Place Module**
- **Tower**

If the **Tower** functional unit of a sample changer version with 2 towers is assigned to the command, the following parameter is also displayed:

Tower	Selection of the tower, with which the command is carried out.

See also

Assigning the lift height (chapter 5.12.3.18.2, page 952)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Defining the lift height (chapter 5.12.3.30.3, page 978)

LIFT – Command variables (chapter 5.11.8.48.1, page 742)

5.11.8.48.1 LIFT – Command variables

The following variables are generated by the **LIFT** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**LiftPosition.Final**.*Command name*' Lift position at the end of the command. Unit: mm

See also

LIFT – Properties (chapter 5.11.8.48, page 738)

5.11.8.49 MOVE TO EXT – Properties

The **MOVE TO EXT** command is used to move to an external position.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*.

In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MOVE TO EXT** command:

Parameters

Target position	Select the position that the robotic arm is to swing to: ▪ **External position** (default value): External position that is defined in the properties of the 786 Swing Head.
Index	Enter the index of the position to which the robotic arm will swing.

Execute with

In order for a **MOVE TO EXT** command to be executed, a functional unit of the **Tower** type needs to be assigned to the command.

If the **Tower** functional unit of a sample changer version with 2 towers is assigned to the command, the following parameter is also displayed:

Tower	Selection of the tower, with which the command is carried out.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

786 Swing Head – Properties (chapter 5.12.3.30.2, page 976)

Command – Directory (chapter 5.11.8.87, page 810)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

MOVE TO EXT – Command variables (chapter 5.11.8.49.1, page 743)

5.11.8.49.1 MOVE TO EXT – Command variables

The following variables are generated by the **MOVE TO EXT** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**PositionType.Final**.*Command name*' Type of the position in which the robotic arm is after the command has been executed (e.g. **external position**). Unit: None
'**PositionIndex.Final**.*Command name*' Index of the position in which the robotic arm is after the command has been executed. Unit: None

See also

MOVE TO EXT – Properties (chapter 5.11.8.49, page 742)

5.11.8.50 MOVE TO RACK – Properties

The **MOVE TO RACK** command is used to move to a specific position on a specific sample rack or the park position.

After selecting the **MOVE TO RACK** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MOVE TO RACK** command:

Parameters

Rack/Park	Select the sample rack on which the position to be approached is: ▪ **Rack** (default value): This substitute value can be defined under **Processes** ▶ **Operating procedure** ▶ **Properties** ▶ **Parameters** in the subsample data as an input field of the **Text** or **Selection list** type to be used as **Rack***(see "Editing subsample data", chapter 5.11.1.10.1, page 404)*. When the command is executed, the value of this input field is automatically applied as the rack name (independently of the input field name). ▪ **Formula**: Define the formula that calculates the rack position. ▪ **Enter value**: Depending on the instrument used, different input options are available. Instruments of the **OMNIS Sample Robot**, **OMNIS Sample Robot NIR** and **OMNIS Sample Robot Oven** types: – **'Rack name'**: Name of the sample rack – **PARK**: Park position – **RP1–RP7**: Absolute rack position **Note**: **RP1**, **RP4** and **RP5** are available rack positions for instruments of the **OMNIS Sample Robot NIR** type. **Note**: **RP1** and **RP2** are available as rack positions for instruments of the **OMNIS Sample Robot Oven** type. Instruments of the **USB Sample Processor** type: – Metrohm recommends entering the article number so that the rack used can be identified unambiguously. – **PARK**: Park position

Position on the rack	Select a sample position on the sample rack: ▪ **Sample position** (default value): This substitute value can be defined under **Processes** ▶ **Operating procedure** ▶ **Properties** ▶ **Parameters** in the subsample data as an input field of the **Number** type to be used as **Sample position** *(see "Editing subsample data", chapter 5.11.1.10.1, page 404)*. When the command is executed, the value of this input field is automatically applied as the sample position. ▪ **Special position**: Position that is defined in the properties of the sample rack as the special position. If **Special position** is selected, then the following specific parameter appears: – **Index** ▪ **Enter position**: Entry of an absolute position on the sample rack. If **Enter position** is selected, then the following specific parameter appears: – **Target position** **Note**: The substitute value **Special position** can only be used with instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**.
Index	Enter the number of the special position (**1–16**). Special positions can be defined under **Equipment** ▶ **Sample racks** ▶ **Properties** ▶ **Positions on the rack** *(see "Defining a special position", chapter 5.12.3.30.4, page 982)*.
Target position	Enter the sample position on the selected sample rack. The position numbers are marked on the sample rack. The number of sample positions on the rack depends on the respective sample rack.

Execute with

In order for a **MOVE TO RACK** command to be executed, one of the following functional units needs to be assigned to the command:

- **Main Module Pick&Place**
- **OMNIS Main Module**
- **Tower**

If the **Tower** functional unit of a sample changer version with 2 towers is assigned to the command, the following parameter is also displayed:

Tower	Selection of the tower, with which the command is carried out.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Defining a special position (chapter 5.12.3.30.4, page 982)

MOVE TO RACK – Command variables (chapter 5.11.8.50.1, page 747)

5.11.8.50.1 MOVE TO RACK – Command variables

The following variables are generated by the **MOVE TO RACK** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**Sampleposition.Final**.*Command name*' ▪ **OMNIS Sample Robot** / **OMNIS Sample Robot NIR** / **OMNIS Sample Robot Oven**: Position on the rack that the gripper arm moves to. ▪ **USB Sample Processor**: Position on the rack that the turntable or robotic arm moves to.
'**Targetposition.Final**.*Command name*' ▪ **OMNIS Sample Robot**: Position (**RP1–RP7**) or designation (**rack name**) of the rack, on which the position moved to by the gripper arm is located, or the park position (**PARK**). ▪ **OMNIS Sample Robot NIR**: Position (**RP1, RP4, RP5**) or designation (**rack name**) of the rack, on which the position moved to by the gripper arm is located, or the park position (**PARK**). ▪ **OMNIS Sample Robot Oven**: Position (**RP1–RP2**) or designation (**rack name**) of the rack, on which the position moved to by the gripper arm is located, or the park position (**PARK**). ▪ **USB Sample Processor**: Designation of the rack (e.g. **article number**) on which the position is moved to or the park position (**PARK**).

See also

MOVE TO RACK – Properties (chapter 5.11.8.50, page 744)

5.11.8.51 MOVE TO WORKSTATION – Properties

The **MOVE TO WORKSTATION** command is used to move the gripper arm to the required workstation and position the gripper above the target position.

After selecting the **MOVE TO WORKSTATION** command, double-clicking on the command or clicking on opens the **Properties** window.

For a **MOVE TO WORKSTATION** command to be executed, 2 functional units of different types need to be assigned to the command in the **Execute with** subsection. The following combinations are possible:

- A functional unit of the **Main Module Pick&Place** type and a functional unit of the **Pick&Place Module** type.
- A functional unit of the **OMNIS Main Module** type and a functional unit of the **Oven Module**, **Pick&Place Module**, **Liquid Sample Presentation** or **Solid Sample Presentation** type.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

MOVE TO RACK – Properties (chapter 5.11.8.50, page 744)

MOVE TO WORKSTATION – Command variables (chapter 5.11.8.51.1, page 748)

5.11.8.51.1 MOVE TO WORKSTATION – Command variables

The following variables are generated by the **MOVE TO WORKSTATION** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command has been stopped, either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that was running in parallel.

Command variables
'**Targetposition.Final**.*Command name*' Workstation that was moved to with the command. ▪ **OMNIS Sample Robot**: **W2**, **W3**, **W5** or **W6** is output as the variable content for the corresponding workstation. Workstations **W1** and **W4** are reserved for pump modules, meaning that they cannot be moved to in order to process samples. ▪ **OMNIS Sample Robot NIR**: **W1** or **W2** is output as the variable content for the corresponding workstation. The workstation for liquid samples is always assigned the designation **W1** and the workstation for solid samples the designation **W2**. ▪ **OMNIS Sample Robot Oven**: **W1** or **W2** is output as the variable content for the corresponding workstation.

See also

MOVE TO WORKSTATION – Properties (chapter 5.11.8.51, page 748)

5.11.8.52 PUMP – Properties

The **PUMP** command is used for controlling a membrane pump or peristaltic pump.

The determination can be held manually during the execution of a **PUMP** command with set pumping duration. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**.

The predefined pumping duration is paused when a time-controlled **PUMP** command is held manually. The pump continues to work during the interruption of the pumping duration. Once the **PUMP** command is continued, the pumping duration continues to run again.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **PUMP** command:

Parameters

Pump control	The pump can be used either in continuous operation or time-controlled: ▪ **On**: The pump remains active until it is switched off with another **PUMP** command or the **Emergency stop function** function. If the determination stops, the pump is only switched off if the **PUMP** command for switching off the pump has been added in the optional run **Execute on stop**. ▪ **Off**: Switch off the pump. ▪ **Time-controlled pumping**: The pump is automatically switched off after the defined **Pumping duration** has elapsed. If the determination stops, the pump is switched off. If **Time-controlled pumping** is selected, the following specific parameter appears: – **Pumping duration**
Pumping duration	Enter the duration (in s) during which pumping should take place.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

For a **PUMP** command to be executed, one of the following functional units needs to be assigned to the command:

- **External Pump Socket**
- **Membrane Pump (Rinse)**
- **Membrane Pump (Aspirate)**
- Peristaltic pump of the **Pump Module**

See also

ADD – Properties (chapter 5.11.8.36, page 701)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

5.11.8.53 ROTATE – Properties

The **ROTATE** command is used to rotate the turntable of the oven module to a specific position.

After selecting the **ROTATE** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **ROTATE** command:

Parameters

Target position	Select the position to which the turntable is rotated. ▪ **Handover position**: The vial cradle is located under the vial holder. ▪ **Analysis position**: The recess at the turntable is located under the vial holder. ▪ **Conditioning position**: The conditioning tube is located under the vial holder. This position may be activated only if the vial holder does not contain a vial.

Additional information on the parameters (e.g., input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **ROTATE** command to be executed, a functional unit of the **Oven Module** type needs to be assigned to the command.

See also

Command – Directory (chapter 5.11.8.87, page 810)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

ROTATE ANGLE – Command variables (chapter 5.11.8.54.1, page 752)

5.11.8.53.1 ROTATE – Command variables

The following variables are generated by the **ROTATE** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**TurntablePosition.Final**.*Command name*' Position where the turntable of the oven module is located after the execution of the command.

See also

ROTATE – Properties (chapter 5.11.8.53, page 750)

5.11.8.54 ROTATE ANGLE – Properties

The **ROTATE ANGLE** command is used for rotating the sample rack by a relative angle.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **ROTATE ANGLE** command:

Parameters

Relative angle	Enter the relative angle (in °) by which the sample rack is rotated starting from the current position.
Rotation rate	Enter the rate (in °/s) at which the sample rack is rotated.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **ROTATE ANGLE** command to be executed, a functional unit of the **Tower** type needs to be assigned to the command.

See also

Command – Directory (chapter 5.11.8.87, page 810)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

ROTATE ANGLE – Command variables (chapter 5.11.8.54.1, page 752)

5.11.8.54.1 ROTATE ANGLE – Command variables

The following variables are generated by the **ROTATE ANGLE** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**AbsoluteAngle.Final**.*Command name*' Absolute angle of the position where the sample rack is after the execution of the command. Unit: °

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

See also

ROTATE ANGLE – Properties (chapter 5.11.8.54, page 752)

5.11.8.55 SLIDE – Properties

The **SLIDE** command is used to move the slide on the Pick&Place module into the exchange position (front) or the work position (rear).

This command can only be executed if the lift on the Pick&Place module is in the top position (0 mm), as otherwise an error message will appear.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **SLIDE** command:

Parameters

Slide position	Target position of the slide: ▪ **Front**: If the slide is at the front, then a sample beaker can be inserted or removed in the front sample position. The storage beaker is to be found in the rear sample position under the titration head. ▪ **Back**: If the slide is at the rear, then the sample beaker is under the titration head.
Speed	Speed at which the slide moves.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **SLIDE** command to be executed, a functional unit of the **Pick&Place Module** type needs to be assigned to the command.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

LIFT – Properties (chapter 5.11.8.48, page 738)

5.11.8.56 STIR – Properties

The **STIR** command is used for stirring with a magnetic stirrer or a rod stirrer.

The determination can be held manually during the execution of a **STIR** command with set stirring time. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **STIR** command:

Parameters

Stirrer control	The stirrer can be used either in continuous operation or time-controlled: ▪ **On**: The stirrer remains activated until a **STIR** command for switch off is issued. If the determination stops, the stirrer is only switched off if the **STIR** command for switching off the stirrer has been added in the optional run **Execute on stop**. ▪ **Off**: Switches the stirrer off. ▪ **Time-controlled stirring**: The stirrer is switched off automatically after the defined stirring time has elapsed. If **Time-controlled stirring** is selected, the following specific parameter appears: – **Stirring time**
Stirring time	Enter the time during which stirring should take place.
Stirring rate	Enter the stirring level and rotation direction of the stirrer. The following values can be entered: ▪ **+1** to **+15**: Stirring levels if the rotation direction of the stirrer is counterclockwise. ▪ **–1** to **–15**: Stirring levels if the rotation direction of the stirrer is clockwise. ▪ **0**: Switch off stirrer. ***Note:*** Metrohm recommends to activate the **Off** selection in the **Stirrer control** parameter to deactivate the functional unit.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

For a **STIR** command to be executed, one of the following functional units needs to be assigned to the command:

- **Magnetic Stirrer**
- **OMNIS Rod Stirrer**
- **Tower Stirrer Socket**
- **801 Stirrer**
- **803 Ti Stand**
- **804 Ti Stand**

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

5.11.8.57 SWING ANGLE – Properties

The **SWING ANGLE** command is used to swing the robotic arm by a relative angle or to an absolute angle.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **SWING ANGLE** command:

Parameters

Swing mode	Select the mode with which the robotic arm is to swing: ▪ **Relative angle**: Relative angle by which the robotic arm is swiveled from the current position. ▪ **Absolute angle**: Absolute angle to which the robotic arm is swiveled.
Angle	Depending on your selection, enter the relative angle by which the robotic arm is swiveled from the current position or enter the absolute angle to which the robotic arm is swiveled.
Swing rate	Enter the rate (in °/s) at which the robotic arm is swiveled.

Execute with

In order for a **SWING ANGLE** command to be executed, a functional unit of the **Tower** type needs to be assigned to the command.

If the **Tower** functional unit of a sample changer version with 2 towers is assigned to the command, the following parameter is also displayed:

Tower	Selection of the tower, with which the command is carried out.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Command – Directory (chapter 5.11.8.87, page 810)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

SWING ANGLE – Command variables (chapter 5.11.8.57.1, page 756)

5.11.8.57.1 SWING ANGLE – Command variables

The following variables are generated by the **SWING ANGLE** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**AbsoluteAngle.Final**.*Command name*' Absolute angle of the position where the robotic arm is after the execution of the command. Unit: °
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

See also

SWING ANGLE – Properties (chapter 5.11.8.57, page 755)

5.11.8.58 PARK LID – Properties

The **PARK LID** command is used to place the sample beaker lid of a sample beaker onto the lid tray. This sample beaker lid is used later to seal the sample beaker with the **RETRIEVE LID** command.

The following conditions must be met to carry out a **PARK LID** command:

- The **sample robot** must be configured for the use of the lid tray.
- The **lid tray** must be mounted and the park positions must be defined.
- The **gripper arm** of the sample robot must be positioned over the active Pick&Place module.
- The **gripper fingers** must hold a sample beaker lid.

After selecting the **PARK LID** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In order for a **PARK LID** command to be executed, a functional unit of the **Main Module Pick&Place** or **OMNIS Main Module** type needs to have been assigned to it beforehand in the **Execute with** subsection.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

5.11.8.59 RETRIEVE LID – Properties

The **RETRIEVE LID** command is used to retrieve a lid from the lid tray with which a sample beaker is then sealed.

The following conditions must be met to carry out a **RETRIEVE LID** command:

- The **sample robot** must be configured for the use of the lid tray.
- The **lid tray** must be mounted and the park positions must be defined.

After selecting the **RETRIEVE LID** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **RETRIEVE LID** command:

Parameters

Lift height	Lift height at which the sample beaker is gripped in the Pick&Place module. This parameter is needed for the lid that was retrieved from the lid tray to be placed correctly on the sample beaker in the Pick&Place module.

The lift height of the sample beaker must be specified. The OMNIS Software takes the thickness of the lid automatically into account.

Additional information on the parameters (e.g., input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **RETRIEVE LID** command to be executed, a functional unit of the **Main Module Pick&Place** or **OMNIS Main Module** type and a functional unit of the **Pick&Place Module** type need to be assigned to it.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

5.11.8.60 FLOW – Properties

The **FLOW** command is used for setting the carrier gas flow of the gas flow unit.

After selecting the **FLOW** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **FLOW** command:

Parameters

Carrier gas flow	Switch the carrier gas flow on or off. If **On** is selected, then the following specific parameters are displayed: ▪ **Flow rate** ▪ **Carrier gas inlet** ▪ **Carrier gas** If **Off** is selected, no further parameters are displayed.
Flow rate	Rate (in mL/min) at which the carrier gas is delivered.
Carrier gas inlet	Selection of the carrier gas inlet: ▪ **Pump** (default value) Ambient air is used as carrier gas. ▪ **Valve** Pressurized gas from a gas bottle is used as carrier gas.
Carrier gas	Selection of the carrier gas used: ▪ **Air** (default value) ▪ **Nitrogen**

Additional information on the parameters (e.g., input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **FLOW** command to be executed, a functional unit of the **Gas Flow Unit** type needs to be assigned to the command.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Gas Flow Unit – Manual control (chapter 5.12.3.19.2, page 955)

KFC – Properties (chapter 5.11.8.11, page 586)

TEMP – Properties (chapter 5.11.8.61, page 759)

5.11.8.61 TEMP – Properties

The **TEMP** command is used for setting the temperature of the oven unit.

The **TEMP** command replaces the **HEAT** command. This command is no longer available in the library starting with Release 2.12.0. Existing methods that contain this command can still be executed and are listed in a message after starting the OMNIS Software so that they can be adjusted.

After selecting the **TEMP** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **TEMP** command:

Parameters

Temperature control	Switch the temperature control on or off. If **On** is selected, then the following specific parameters are displayed: ▪ **Temperature control mode** ▪ **Target temperature**

Temperature control mode	Selection of the temperature control type: ▪ **Fixed target temperature** The target temperature is reached as quickly as possible. ▪ **Gradient** The target temperature is reached with the predefined gradient. If **Gradient** is selected, then the following specific parameter is displayed: ▪ **Temperature gradient**
Target temperature	Temperature to which the oven is to be regulated. Depending on the current temperature and the target temperature, the oven is heated up or cooled down.
Temperature gradient	Starting with the current oven temperature, the target temperature is to be reached with the defined temperature gradient.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

Execute with

In order for a **TEMP** command to be executed, a functional unit of the **Oven Unit** type needs to be assigned to the command.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

FLOW – Properties (chapter 5.11.8.60, page 758)

KFC – Properties (chapter 5.11.8.11, page 586)

Oven Unit – Manual control (chapter 5.12.3.19.1, page 954)

5.11.8.62 TRANSPORT OVEN VIAL – Properties

The **TRANSPORT OVEN VIAL** command is used to transport the vial from the vial cradle to the oven for analysis or from the oven back to the vial cradle after analysis.

After selecting the **TRANSPORT OVEN VIAL** command, double-clicking on the command or clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **TRANSPORT OVEN VIAL** command:

Parameters

Vial target position	Select the vial target position: ▪ **Analysis**: The vial is in the oven after the command sequence has been run. The analysis can be started. ▪ **Handover**: The vial is in the vial cradle after the command sequence has been run. From here, the vial is transferred to the robot arm of the main module.
Lift rate	Speed at which the lift is to be moved. The **Maximum** default value is selected.

Execute with

In order for a **TRANSPORT OVEN VIAL** command to be executed, a functional unit of the **Oven Module** type needs to be assigned to the command.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

5.11.8.63 ADD TO SAMPLE LIST – Properties

Information on the **ADD TO SAMPLE LIST** command in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The **ADD TO SAMPLE LIST** command is used to automatically add samples and subsamples to the sample list during the determination.

After selecting the **ADD TO SAMPLE LIST** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. The following functions and information are available for the **ADD TO SAMPLE LIST** command in the **Parameters** subsection:

Samples/subsample definition

Add to the sample list	Select whether a sample with associated subsamples or only subsamples are added. ▪ **Sample**: A new sample with subsamples can be defined and added to the sample list. If **Sample** is selected, then the following button appears: – **Define sample/subsamples** ▪ **Subsamples**: One or more subsamples can be defined and added to the sample list within the current sample. If **Subsamples** is selected, then the following button appears: – **Define subsamples**
Define sample/subsamples	Window for defining a sample and its subsamples that are added to the sample list: *Additional information*
Define subsamples	Window for defining subsamples that are added to the sample list within the current sample: *Additional information*
Insertion position	
Position in the sample list	Select the position at which the sample or subsamples are to be inserted in the sample list. ▪ **At the end of the current sample**: If a new sample is added, then it is inserted directly after the sample for which this command is executed. If subsamples are added to the current sample, then these are inserted at the end of the sample. ▪ **After the current subsample**: The sample or the subsamples are inserted directly after the subsample for which this command is executed. ▪ **At the end of the sample list**: The sample or the subsamples are inserted at the end of the sample list. Additional information on the insertion behavior of the sample or subsamples: *(see "ADD TO SAMPLE LIST – Principle", chapter 5.11.8.63.1, page 766)*
Subsample status	
Status selection	Select the status that the added subsamples have. ▪ **Waiting for execution**: The subsamples have the **Waiting for execution** status and are added to the current series or parallel determination. If the subsample for which this command is executed is analyzed as a single determination, then the new subsamples are added to the **Ready** status. ▪ **Ready**: The added subsamples have the **Ready** status. ▪ **Ready with planned determination**: The added subsamples have the **Ready with planned determination** status and their determination is started after the defined delay. If **Ready with planned determination** is selected, then the following specific parameters appear: – **Delay of the determination start** – **Determination type**

Delay of the determination start	The start of the determination of the subsamples is delayed by the defined time, starting from when it is added to the sample list.
Determination type	Select determination type of the subsamples. The determination type is used if no determination is running at the time of the determination start of the added subsamples. ▪ **Series determination**: The added subsamples are analyzed consecutively. ▪ **Parallel determination**: The added subsamples are analyzed in parallel. **Notice:** If a determination series is already running at the time the of the determination start, then the subsamples are added to the current determination series and the existing determination type is applied. If a single determination is running at the time of the determination start, then the subsamples are not executed and are assigned the **Ready** status.

Defining a sample and subsamples

The following functions and information are available in the **Define sample/subsamples** and **Define subsamples** windows, depending on the selection in the **Add to the sample list** parameter. Additional information on the icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

Sample

Sample profile	If sample data is to be used for the added sample, then a sample profile can be selected from the selection list. The sample data is applied from the selected sample profile according to the following rules and can then be edited in the command parameters: ▪ The sample data is applied with its default values. ▪ The input ranges and properties defined in the sample profile apply to the input fields. ▪ If the **Force entry** check box is enabled in the sample profile, then the input field can be left empty only if the subsamples are added to the sample list in the **Ready** status. ▪ Non-editable input fields and input fields with the **Result** usage type are not displayed. ▪ The operating procedures and number of subsamples defined in the sample profile are not taken into account. If **Default value** is selected for the sample data, then the default value defined in the sample profile is always used. This also applies if it is changed after the command has been parameterized. **Notice:** The formula function can be used to apply sample data from the sample for which the **ADD TO SAMPLE LIST** command is being executed. For example, the name of the sample as part of the name of the new sample. **Notice:** If the sample data in the referenced sample profile is changed after the parameterization of the **ADD TO SAMPLE LIST** command, then these changes must also be applied in the command. Otherwise, the operating procedure containing the command can no longer be executed. To apply the changes, the operating procedure or the method containing the command must be opened and the parameters updated based on the message that appears. The changed input fields and their values should then be checked again. The sample data can no longer be changed once the operating procedure or the method that contains the **ADD TO SAMPLE LIST** command has been published. Changes to the sample profile no longer affect the command and its execution capability.
Name	Enter the name of the sample. If a sample profile is used, then the name of the sample is applied from the default value in the sample profile and can then be edited.
Subsample 1–25	

Operating procedure	Select the required operating procedure from the selection list that is used for the added subsample. The subsample data is applied from the selected operating procedure according to the following rules and can then be edited in the command parameters: ▪ The subsample data is applied with its default values. ▪ The input ranges and properties defined in the operating procedure apply to the input fields. ▪ If the **Force entry** check box is enabled in the operating procedure, then the input field can be left empty only if the subsamples are added to the sample list in the **Ready** status. ▪ Non-editable input fields and input fields with the **Result** usage type are not displayed. If **Default value** is selected for the subsample data, then the default value defined in the operating procedure is always used. This also applies if it is changed after the command has been parameterized. **Notice:** The formula function can be used to apply subsample data from the subsample for which the **ADD TO SAMPLE LIST** command is being executed. For example, the name of the subsample as part of the name of the new subsample or the dilution of the subsample to calculate the dilution for the new subsample. **Notice:** If the subsample data in the referenced operating procedure is changed after the parameterization of the **ADD TO SAMPLE LIST** command, then these changes must also be applied in the command. Otherwise, the operating procedure containing the command can no longer be executed. To apply the changes, the operating procedure or the method containing the command must be opened and the parameters updated based on the message that appears. The changed input fields and their values should then be checked again.
Name	Enter the name of the subsample. The name of the subsample is applied from the default value in the operating procedure and can then be edited.

When this command is executed, subsamples are automatically created and started by the system. This can be traced in the sample list in the **Subsample** ► **History** area as follows:

- The user **System** is displayed for the parameters **Created by**, **Saved by** and **Started by**.
- The object ID of the subsample for which the **ADD TO SAMPLE LIST** command was executed is displayed for the parameters **Creation triggered by subsample** and **Start triggered by subsample**.

The subsamples defined in the **ADD TO SAMPLE LIST** command are already checked for the conditions for successful execution during the manual and preliminary run test for the subsample that contains the operating procedure with the **ADD TO SAMPLE LIST** command. Additional information on the run test: *(see "Run test – Brief description", chapter 5.10.8.1, page 295)*

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

ADD TO SAMPLE LIST – Principle (chapter 5.11.8.63.1, page 766)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Recording samples (chapter 5.10.4.1, page 251)

Recording subsamples (chapter 5.10.7.1, page 273)

5.11.8.63.1 ADD TO SAMPLE LIST – Principle

Insertion behavior

Use the **ADD TO SAMPLE LIST** command to add samples and subsamples automatically to the sample list during the determination. Depending on the parameterization of the command, the sample or subsamples are inserted in the sample list as follows:

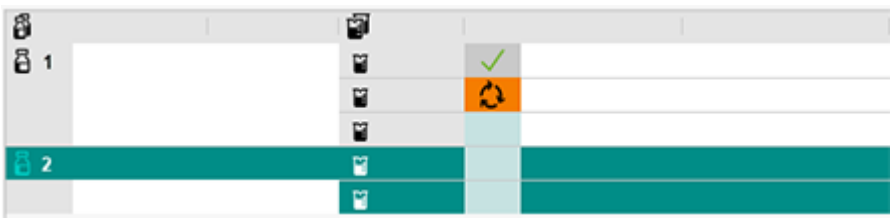
New sample

Parameterization:

- Add to the sample list: **Sample**
- Position in the sample list:

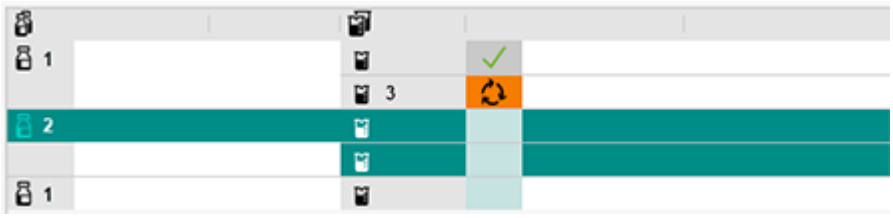
At the end of the current sample

The new sample (2) is inserted directly after the sample (1) that contains the subsample for which the **ADD TO SAMPLE LIST** command is executed.



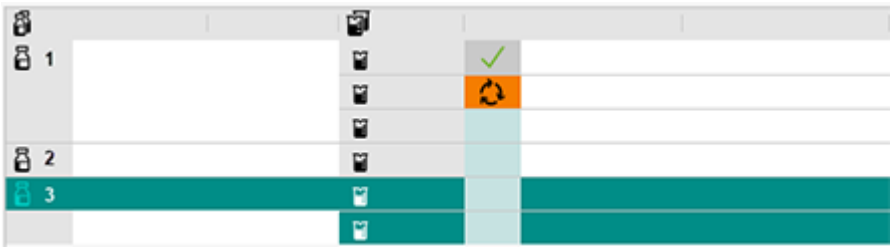
After the current subsample

The new sample (2) is inserted directly after the subsample (3) for which the **ADD TO SAMPLE LIST** command is executed. The sample (1) is split into several parts if it contains further subsamples after the current subsample.



At the end of the sample list

The new sample (3) is inserted at the end of the sample list, after all other samples contained there (1, 2).



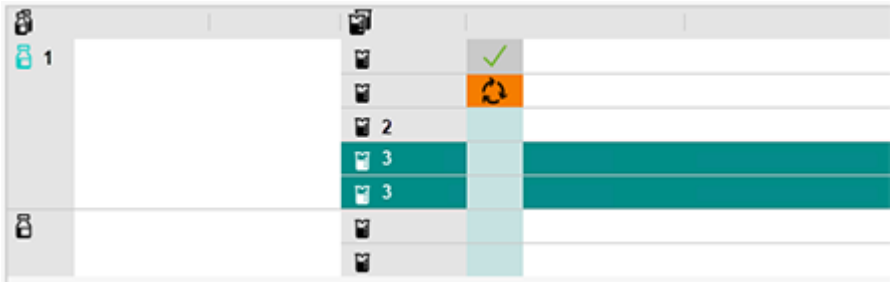
New subsamples in existing sample

Parameterization:

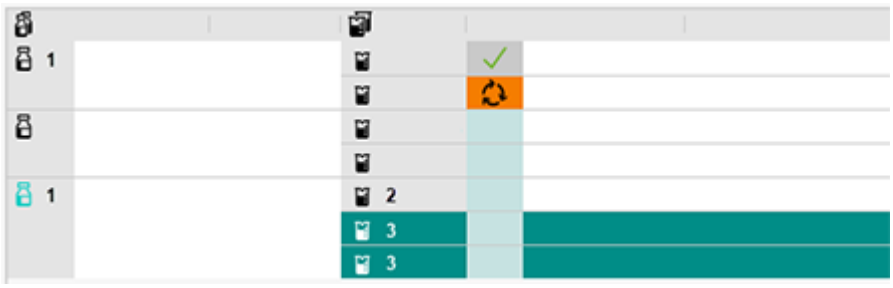
- Add to the sample list: **Subsamples**
- Position in the sample list:

At the end of the current sample

The new subsamples (3) are inserted after the last subsample (2) of sample (1). The subsamples are inserted in the sample for which the **ADD TO SAMPLE LIST** command is executed.

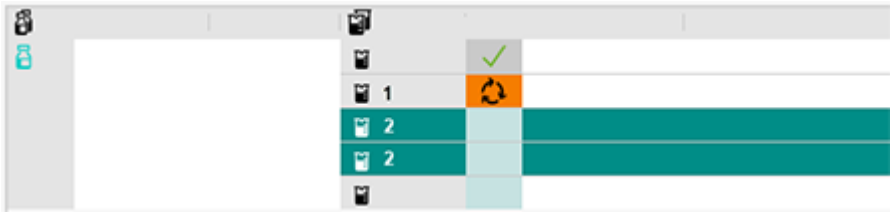


If the sample (1) is split into several parts, then the new subsamples (3) are inserted after the last subsample (2) of the sample in the sample list.



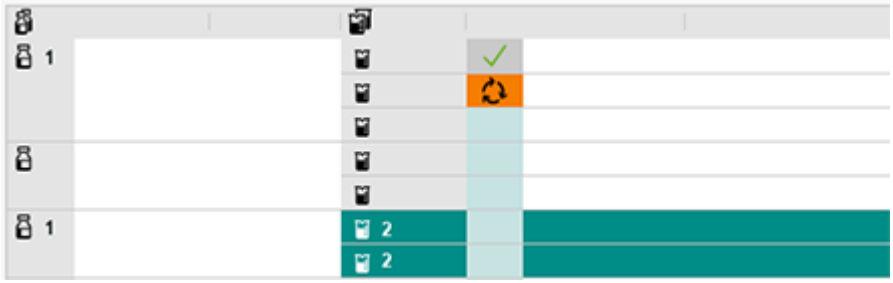
After the current subsample

The new subsamples (2) are inserted directly after the subsample (1) for which the **ADD TO SAMPLE LIST** command is executed.



At the end of the sample list

The new subsamples (2) are inserted at the end of the sample list. If the sample (1) for which the **ADD TO SAMPLE LIST** command is executed is not at the end of the sample list, then it is split into multiple parts.



See also

ADD TO SAMPLE LIST – Properties (chapter 5.11.8.63, page 761)

5.11.8.64 CALC – Parameters

The **CALC** command is used for calculating results. The required formula can be created using the formula editor.

Only one result can be calculated per **CALC** command. If several results should be calculated, then several commands have to be added.

In the OMNIS Software version 2.11.0, **CALC** commands can only write on sample data and subsample data that has been defined as **Result**. Operating procedures containing invalid variables can no longer be executed. If such an operating procedure is started, the affected **CALC** commands are listed in an error message. For a successful determination of a subsample, the relevant **CALC** commands must be manually adjusted.

The **CALC** command is executed with the following parameters:

Result name	Name of the result, which is shown in **Results** ▶ **Calculations** and in the report.
Result unit	Unit that is displayed together with the result. The selected unit has no influence on the calculation and is used exclusively for displaying the result in the formula editor's result field, in reports and in the result monitoring.
Decimal places	Number of decimal places to which the result is rounded. The number of decimal places specified only applies for displaying the result. The result is saved with maximum accuracy and used in additional calculations regardless of the setting.
Formula	Formula used for the calculation of the result. Clicking on f_x opens the formula editor, which can be used to define or edit a calculation formula.
Save result in variable	Variable used for saving the result. Clicking (x) opens a dialog window in which the desired variable can be selected from existing variables of the following variable categories: ▪ **Sample data**: Selection of the sample data that was defined as result in the sample profile. ▪ **Subsample data**: Selection of the subsample data that was defined as result in the operating procedure. ▪ **Method variables**: Selection of the method variables defined in the method. ▪ **System variables**: Selection of the system variables defined in the sample area.
Calculate statistics	If the check box is activated, the statistics values for the results are calculated and displayed.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

CALC – Command variables (chapter 5.11.8.64.1, page 770)

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Editing subsample data (chapter 5.11.1.10.1, page 404)

Formula editor – Brief description (chapter 5.11.9, page 825)

Monitoring – Definition (chapter 5.10.13.4, page 355)

NOTIFY – Parameters (chapter 5.11.8.72, page 787)

REQUEST – Parameters (chapter 5.11.8.77, page 794)

Reprocessing subsample data (chapter 5.10.7.5, page 283)

Result monitoring – Definition (chapter 5.11.1.11, page 408)

5.11.8.64.1 CALC – Command variables

The following variables are generated by the **CALC** command during the process sequence and can be used in a formula under the '**Result name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'*Result name*.*Command name*'

Result value of the calculation. No further statistics is calculated here.

Unit: Determined in the **Result unit** field

'**MeanValue**.*Result name*.*Command name*'

Mean value of all results that have already been determined with the same operating procedure version and with the same method versions before.

'**StandardDeviation**.*Result name*.*Command name*'

Absolute standard deviation of the result. The values of the current subsample and of all subsamples that have already been determined with the same operating procedure version and with the same method versions before are used for the calculation.

See also

CALC – Parameters (chapter 5.11.8.64, page 768)

Formula editor – Brief description (chapter 5.11.9, page 825)

NOTIFY – Parameters (chapter 5.11.8.72, page 787)

5.11.8.65 CALL WEB API - Parameter

The **CALL WEB API** command is used to send data to a web API for further use in third-party software.

The **CALL WEB API** command is executed with the parameters listed in the following:

API endpoint URL	URL (web address) that leads to the web API endpoint. The endpoint refers to the hostname of the web API. Example for an API endpoint URL: https://api.beispiel-server.com/measurementdata
[Edit Request Body]	The window for defining the Request Body is opened. The Request Body is sent via the HTTP method **POST** to the web API. The input can contain formulas and must conform to a valid JSON (JavaScript Object Notation) format. Clicking f_x opens the formula editor, which can be used to insert variables and formulas for the Request Body. **Note**: When using variables, the correct use of parentheses at the beginning and end of each variable must be observed. A clicking 3 times on an inserted variable highlights the whole variable, including its parentheses.

Authentication type	Select the authentication type for the access to the web API: ▪ **None** ▪ **Basic** ▪ **OAuth2** If **Basic** is selected, the following specific parameters appear: ▪ **User name** ▪ **Password** If **OAuth2** is selected, the following specific parameters appear: ▪ **User name** ▪ **Password** ▪ **Token URL** ▪ **Client ID** ▪ **Client Secret** ▪ **Scope**
User name	Enter the user name for the access to the web API.
Password	Enter the password that authorizes the user to access the web API.
Token URL	Enter the web address via which the access token for the authentication on the web API is requested.
Client ID	Enter client ID assigned by the authorization server. The client ID is a publicly available character string and is used to identify the application.
Client Secret	Enter secret client key assigned by the authorization server. The client key is used to authenticate the identity of the application to the Web API.
Scope	Enter the scope granted by the access token for the web API.
Cancel after error	If this check box is enabled, the determination is aborted after an error and the subsample receives the **Canceled after error** status. If this check box is disabled, the subsample receives the **Completed** status in case of an error and the determination is continued.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

5.11.8.66 CONSUME SUBSAMPLE – Consume subsample

With the **CONSUME SUBSAMPLE** command, the user can determine from which point in the run a subsample is considered consumed.

If the run is stopped (stop, emergency stop or stop by error) before the **CONSUME SUBSAMPLE** command was processed, the subsample is not considered to be consumed, i.e. it can be started again. All results and measuring point lists are discarded, but the sample data and subsample data are retained.

If the run is stopped after the **CONSUME SUBSAMPLE** command was processed, the subsample is considered consumed, i.e. it has to be recorded again for a new analysis. If the run is stopped after the **CONSUME SUBSAMPLE** command was processed, the subsample is considered consumed and it is highlighted as not completed (e.g. as **Canceled after stop** or **Canceled after error**). The subsample must either be reset to status **Ready** or a new subsample must be registered for it to be analyzed again.

If no **CONSUME SUBSAMPLE** command is present in the run, then the subsample is considered to be consumed as soon as the determination starts.

Hint

It is recommended to insert the **CONSUME SUBSAMPLE** command if subsamples are only used later on in the determination run, i.e. for analysis with a sample robot or Karl Fischer titration with conditioning.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Conditioning – Principle (chapter 5.11.8.10, page 567)

Creating and editing a method (chapter 5.11.3.3, page 418)

KFT – Command variables (chapter 5.11.8.10.3, page 582)

KFT – Properties (chapter 5.11.8.10.1, page 568)

Karl Fischer titration – Principle (chapter 5.11.8.9, page 561)

5.11.8.67 EVAL BASE STATISTICS – Parameters

The **EVAL BASE STATISTICS** command is used to statistically evaluate the selected quantity of a measuring point list. The results **First value**, **Integral value** (only **MEAS SPEC**), **Least value**, **Maximum value**, **Minimum value**, **Mean value** and **Standard deviation** are generated. Preprocessing measures can be defined, depending on the referenced command.

In the method, the referenced command must be executed **before** the **EVAL BASE STATISTICS** command.
The **EVAL BASE STATISTICS** command can now reference the following commands: **MEAS SPEC**, **COLLECT**.

The **EVAL BASE STATISTICS** command is executed with the parameters listed in the following:

Name of the command	Selection of the command from the measuring point list of which a statistical evaluation is to be performed on the selected quantity. If a **MEAS SPEC** command is selected, then the following specific buttons appear: ▪ **[Define data preprocessings]** ▪ **[Define wavelength ranges]**. If a **COLLECT** command is selected, then the following specific parameter appears: ▪ **Quantity**
[Define data preprocessings]	The subsection for defining the data preprocessing is opened. More information on data preprocessing and the associated parameters: *(see "Data preprocessing – Area", chapter 5.13.1.17, page 1100)*
[Define wavelength ranges]	The subsection for defining the wavelength ranges is opened. Additional information on wavelength ranges and the associated parameters: *(see "Wavelength range – Area", chapter 5.13.1.18, page 1102)*
Quantity	Selection of a quantity of the **COLLECT** command via which a statistical evaluation is to be performed.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

COLLECT – Parameters (chapter 5.11.8.12.1, page 602)

Command – Directory (chapter 5.11.8.87, page 810)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

5.11.8.67.1 EVAL BASE STATISTICS – Command variables

The following variables are generated by the **EVAL BASE STATISTICS** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**First.Result**.*Command name*' **MEAS SPEC**: First absorbance value over the defined wavelength ranges. **COLLECT**: First value of the defined measured quantity from the measuring point list.
'**Integral.Result**.*Command name*' **MEAS SPEC**: Integral value of the absorbance values over the defined wavelength ranges. **COLLECT**: Measured value is always invalid.
'**Last.Result**.*Command name*' **MEAS SPEC**: Last absorbance value over the defined wavelength ranges. **COLLECT**: Last value of the defined measured quantity from the measuring point list.
'**Maximum.Result**.*Command name*' **MEAS SPEC**: Maximum absorbance value over the defined wavelength ranges. **COLLECT**: Maximum value of the defined measured quantity from the measuring point list.
'**Mean.Result**.*Command name*' **MEAS SPEC**: Mean value of the absorbance values over the defined wavelength ranges. **COLLECT**: Mean value of the defined measured quantity from the measuring point list.
'**Minimum.Result**.*Command name*' **MEAS SPEC**: Minimum absorbance value over the defined wavelength ranges. **COLLECT**: Minimum value of the defined measured quantity from the measuring point list.
'**StandardDeviation.Result**.*Command name*' **MEAS SPEC**: Standard deviation of the absorbance values over the defined wavelength ranges. **COLLECT**: Standard deviation of the defined measured quantity from the measuring point list.

See also

CALC – Parameters (chapter 5.11.8.64, page 768)

COLLECT – Parameters (chapter 5.11.8.12.1, page 602)

EVAL BASE STATISTICS – Parameters (chapter 5.11.8.67, page 773)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

5.11.8.68 EVAL LINEAR REGRESSION – Parameters

The **EVAL LINEAR REGRESSION** command is used to carry out a linear regression over a measuring point range in the measuring point list of a command or over the results of several subsamples using the least squares method. For the linear regression over several subsamples, the values for the x-axis and y-axis are calculated by referenced **CALC** commands.

The linear regression over a measuring point range in the measuring point list can be used for the following calculations:

- Rate evaluation for the **STAT pH** command and for **STAT U** command: *(see "STAT – Principle", chapter 5.11.8.7, page 533)*
- Post-drift correction for Karl Fischer titrations: *(see "Karl Fischer titration – Principle", chapter 5.11.8.9, page 561), (see "Conditioning – Principle", chapter 5.11.8.10, page 567)*
- Titer determination and blank value determination in thermometric titration: *(see "TET – Principle", chapter 5.11.8.5, page 497)*

In the method, the referenced commands must be executed **before** the **EVAL LINEAR REGRESSION** command. These commands generate the measured values for the regression analysis.

In cases of linear regression via multiple subsamples, neither the **EVAL LINEAR REGRESSION** command nor the **CALC** commands used may be included in a **LOOP** run sequence. Errors in the determination might otherwise occur.

Only valid measured values that lie within the defined evaluation window are taken into account with linear regressions which use a measuring point list. At least 2 valid measured values must be found in the evaluation window to successfully carry out the linear regression.

The **EVAL LINEAR REGRESSION** command is executed with the parameters listed in the following:

Linear regression over	Origin of the data that is to be evaluated for the linear regression: ▪ **Measuring point list**: The data to be evaluated originates from the measuring point list of the referenced command. If **Measuring point list** is selected, the following specific parameters appear after the selection of the referenced command: – **Quantity on the x-axis** – **Lower limit** – **Upper limit** – **Quantity on the y-axis** ▪ **Multiple subsamples**: The data to be evaluated originates from the results of 2 defined calculations in multiple subsamples of a sample which was analyzed with the same version of the operating procedure and method. If **Multiple subsamples** is selected, the following specific parameters appear: – **Data for the x-axis** – **Data for the y-axis**
Name of the referenced command (only for Measuring point list)	Selection of the command that generates the measuring point list to be evaluated.
Quantity on the x-axis (only for Measuring point list)	Independent variable that is to be shown on the x-axis at the time of the evaluation: Only valid for **KFC**: ▪ **Water** Only valid for **KFT Ipol**, **STAT pH** and **STAT U**: ▪ **Volume** Valid for all commands: ▪ **Time**
Lower limit (only for Measuring point list)	Defines the lower limit of the evaluation window. The value of the lower limit is contained in the evaluation window.
Upper limit (only for Measuring point list)	Defines the upper limit of the evaluation window. The value of the upper limit is not contained in the evaluation window.

Quantity on the y-axis (only for Measuring point list)	Dependent variable that is to be shown on the y-axis at the time of the evaluation: Only valid for **KFC**: ▪ **Water** ▪ **Potential** ▪ **Charge** Only valid for **KFT Ipol**: ▪ **Volume** ▪ **Potential** Only valid for **STAT pH**: ▪ **Volume** ▪ **pH** Only valid for **STAT U**: ▪ **Volume** ▪ **Potential** Valid for all commands: ▪ **Time** ▪ **Drift** ▪ **Temperature**
Data for the x-axis (only for Multiple subsamples)	Selection of the **CALC** command with which the values for the x-axis of the data point are to be recorded.
Data for the y-axis (only for Multiple subsamples)	Selection of the **CALC** command with which the values for the y-axis of the data point are to be recorded.

The following values are output under **Sample list** ▶ **Results** ▶ **Raw data** as results of the command:

- Slope
- y-intercept
- Coefficient of determination R^2
- Number of data points

Once the **EVAL LINEAR REGRESSION** command has been selected in the selection list , the following values will be output further:

- Standard error of slope
- Standard error of y-intercept
- Standard error of estimate y
- F statistic
- Degrees of freedom
- Regression sum of squares
- Residual sum of squares

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Command – Directory (chapter 5.11.8.87, page 810)

EVAL LINEAR REGRESSION – Command variables (chapter 5.11.8.68.1, page 779)

STAT – Principle (chapter 5.11.8.7, page 533)

5.11.8.68.1 EVAL LINEAR REGRESSION – Command variables

The following variables are generated by the **EVAL LINEAR REGRESSION** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

Command variables
'**CoefficientOfDetermination.Result**.*Command name*' The coefficient of determination (R^2) as a quality criterion of linear regression. The coefficient of determination indicates how suitable the independent variables are for explaining the variance of the dependent variables.
'**DegreeOfFreedom.Result**.*Command name*' Degrees of freedom as the number of the evaluated data points minus 1.
'**Finished**.*Command name*' Status of the command. ▪ **Invalid**: The command has not been started (yet). ▪ **0**: The command is still running. ▪ **1**: The command has been completed correctly. ▪ **2**: The command has not been completed correctly. An error or a warning occurred. ▪ **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**. ▪ **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.
'**FStatistic.Result**.*Command name*' F statistic as the explained variance in proportion of the unexplained variance of the results. With the F statistic it can be established if the ratio between the dependent and the independent variable is random or not.
'**Intercept.Result**.*Command name*' y-intercept of the linear regression.

Command variables
'**NumberOfDataPoints.Result**.*Command name*' Number of data points that are evaluated for the linear regression. Only measured values that are valid and lie within the defined evaluation window are included.
'**Regression.SumOfSquares.Result**.*Command name*' Regression sum of squares or explained sum of squares of the analysis. The sum corresponds to the variance between the mean value and the estimates that is explained by the regression function.
'**Residual.SumOfSquares.Result**.*Command name*' Residual sum of squares of the analysis. The residues correspond to the difference between the estimate and the actual measured value for each data point.
'**Slope.Result**.*Command name*' Slope of the regression line.
'**StandardError.Intercept.Result**.*Command name*' Standard error of y-intercept.
'**StandardError.Slope.Result**.*Command name*' Standard error of slope.
'**StandardError.YEstimate.Result**.*Command name*' Standard error of estimate y.

See also

CALC – Parameters (chapter 5.11.8.64, page 768)

5.11.8.69 EXPORT – Parameters

The **EXPORT** command is used to export determination data as a CSV file for further use, e.g. in a LIMS (Laboratory Information Management System).

The **EXPORT** command is executed with the parameters listed in the following:

Export type	Selection of the export type with which the determination data is to be exported: ▪ **CSV – Sample data and subsample data** All sample data and subsample data of a determination are exported in the CSV (Comma Separated Value) file format. The exported files contain at least 2 lines that are separated by CR/LF (line break). The top line contains the column headings (**Field name short** for sample data and subsample data). The line below contains the field contents. All fields are separated by the "**;**" character. The order of the fields for the sample data and subsample data corresponds to the order in the sample list. ▪ **CSV – Raw data and results** The measuring point list, the list of the equivalence points or endpoints, the list of the fixed points and the calculation results will be exported in the CSV (Comma Separated Value) file format for each measuring command of a determination. All fields are separated by the "**;**" character. For the results, the result value and result unit are output in 2 separate fields.
Export in	When exporting sample data and subsample data, the determination data can be added to an existing CSV file or it can be exported in separate files. ▪ **One file**: The collective determination data of all analyzed subsamples is exported in one file. If the file does not exist yet, it is created. If the file already exists, the new determination data is added. If samples are exported that have different column headings, a column heading is only then written new if it differs from the previous one. ▪ **Separate files**: The determination data is exported for each subsample in one individual file with a unique name.
Target folder	Folder where the export file is saved. The following options are available: ▪ Select a target folder by clicking on . ▪ Enter the absolute path (e.g. **C:\Users\Public\Documents\OMNIS\...**). ▪ An existing target folder can be supplemented with a new subfolder. This is created by the OMNIS Software.
File name	File name under which the file is saved. The following options are available: ▪ Enter the text; the following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9 ▪ Enter the file name using the formula editor and variable. When exporting in separate files, the file name is appended automatically with the date and time in the **-YYYY-MM-DD-hh-mm-ss-ms** format (e.g. **-2017-02-14-08-02-07-549**).

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Operating procedure – Properties (chapter 5.11.1.2, page 383)

5.11.8.70 IF – Parameters

The **IF** command is used to execute a part of a process (operating procedure or method) only if a defined condition is met.

The **IF** command is executed with the following parameters:

Condition	Display of the condition for the execution of the sequence of commands and methods contained in the command: ▪ If the condition is met, the run defined in the **IF** command is executed. The process then continues to run as defined in the process editor. ▪ If the condition is not met, the run defined in the **IF** command is not executed. The process then continues to run as defined in the process editor. Clicking on f_x opens the formula editor, which can be used to define or edit the condition. If an error occurs while calculating the condition, the **IF** command is skipped and the process is continued as defined in the process editor.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

IF – Concept (chapter 5.11.8.70.1, page 783)

NOTIFY – Parameters (chapter 5.11.8.72, page 787)

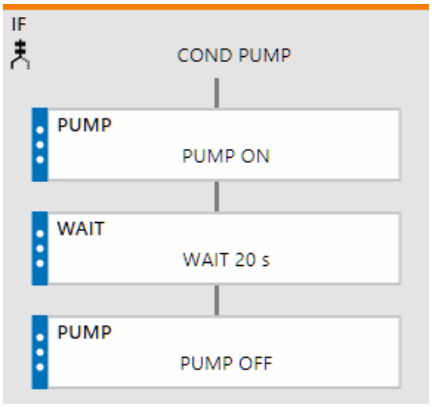
5.11.8.70.1 IF – Concept

Structure

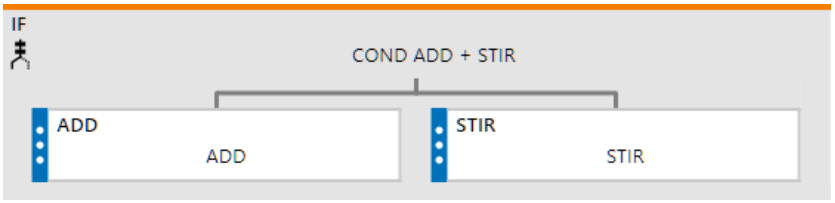
The **IF** command can be used to define a run of commands and methods that are then carried out only if the condition defined in the **IF** command is met.

In these runs, serial and parallel process sequences are displayed as follows:

- **Serial sequence**



- **Parallel sequence**



Representation in operating procedures and methods

Clicking on ❯ shows the run with its commands and methods in a separate area. Clicking on ❮ closes the separate area again. The icon next to the arrow displays the following:

❮□ The IF run does not contain any commands.

❮■ The IF run contains commands.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

IF – Parameters (chapter 5.11.8.70, page 782)

NOTIFY – Parameters (chapter 5.11.8.72, page 787)

5.11.8.71 LOOP – Parameters

The **LOOP** command is used to create a run sequence of commands and methods which can be repeated multiple times.

The **LOOP** command is executed with the parameters listed in the following:

The parameters represent 3 possible exit conditions, which are checked from top to bottom. The exit condition that is reached first leads to the end of the run sequence.
At least one parameter must be defined.

Maximum number of runs	Maximum number of repetitions for the run sequence of commands and methods defined in the **LOOP** command. If the specified maximum number of runs has been reached, then the run sequence will be ended the next time the **LOOP** command is called. The parameter is always checked at the start of each run. If a formula is defined for the **Maximum number of runs** parameter, and an error occurs when calculating the formula, then the **LOOP** command is skipped and the process sequence is continued.
Maximum duration	Maximum expiry time of the **LOOP** command. If the specified maximum duration is reached, then the current run sequence will nevertheless continue to run through to the end. The **LOOP** command is then ended. The parameter is always checked at the start of each run.
Condition	Exit condition for the run sequence of commands and methods defined in the **LOOP** command. Clicking on f_x opens the formula editor, which can be used to define or edit the condition. If the condition is fulfilled (evaluation of the formula yields the result 1 = true), then the run sequence will be ended when the **LOOP** command is called again. The parameter can be checked at the start or end of a run. The run sequence is run at least once during the check at the end of the run. If an error occurs while calculating the condition, then the **LOOP** command is skipped and the process is continued as defined in the process editor.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

LOOP – Command variables (chapter 5.11.8.71.2, page 786)

LOOP – Concept (chapter 5.11.8.71.1, page 785)

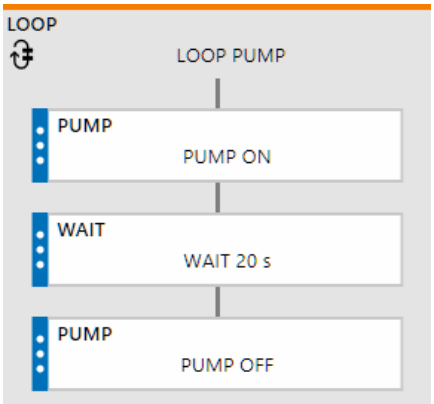
5.11.8.71.1 LOOP – Concept

Structure

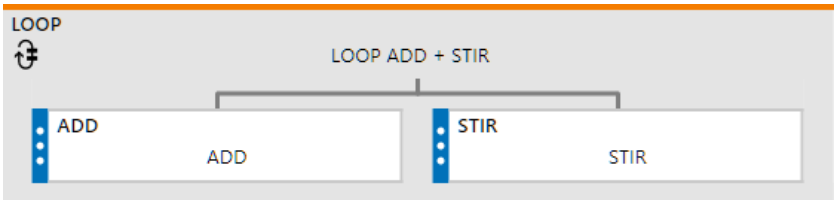
The **LOOP** command can be used to define a run sequence of commands and methods that can be carried out repeatedly.

Serial and parallel process sequences are displayed as follows in these run sequences:

- **Serial run**



- **Parallel run**



Depiction in operating procedures and methods

Clicking on ❯ shows the run sequence with its commands and methods in a separate area. Clicking ❮ closes the separate area again. The symbol next to the arrow indicates the following:

❯□ The run sequence defined in the **LOOP** command does not contain any commands.

❯■ The run sequence defined in the **LOOP** command contains commands.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

LOOP – Command variables (chapter 5.11.8.71.2, page 786)

LOOP – Parameters (chapter 5.11.8.71, page 784)

5.11.8.71.2 LOOP – Command variables

The following variables are generated by the **LOOP** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

'**Duration**.*Command name*'

Total duration for the processing of the command.

Unit: s

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual user intervention (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**LoopCount**.*Command name*'

Number of run sequences of the **LOOP** command that have been run.

'**LoopFinish**.*Command name*'

Information status about the end of the command.

- **Invalid**: The command is still running. An error or a warning occurred.
- **1**: The maximum number of runs has been reached.
- **2**: The maximum duration of the **LOOP** command has been reached.
- **3**: The condition has been fulfilled.

See also

LOOP – Concept (chapter 5.11.8.71.1, page 785)

LOOP – Parameters (chapter 5.11.8.71, page 784)

5.11.8.72 NOTIFY – Parameters

Information on the settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The **NOTIFY** command is used to send an e-mail notification via the OMNIS Software. The notification text can be created by the sender using the text editor.

To be able to use the **NOTIFY** command, first, all of the notification settings must be implemented under **Settings** ▶ **General settings** and a connection to the email server must be set up. Additional information on notification settings: *(see "Setting up notifications", chapter 5.15.1, page 1199)*

The **NOTIFY** command can be used in combination with other commands (e.g. optional run **Execute on limit**, **IF** command) to dispatch an automatic notification when a particular event occurs. In the event of a limit value violation, the **NOTIFY** command provides information, e.g. on the violation of at least one limit value and supplies necessary information regarding result monitoring.

There is a risk of triggering an endless number of notifications when the **NOTIFY** command is used in combination with a **LOOP** command.

The **NOTIFY** command is executed with the parameters listed in the following:

Subject	Subject line of the notification. If the field remains empty, then the notification is dispatched without a subject.
Recipient	E-mail address of the notification recipient. The e-mail address must have the following format: name@example.com Multiple email addresses can be entered. These must be separated from one another with a semicolon **(;)**.

[Edit notification]

Open the text editor for creating and editing the notification. The notification defined here is dispatched to the recipient(s) as an email at the time the command is executed.

Clicking (x) opens a dialog window where a variable can be inserted into a notification as placeholder text. When the notification is sent, the variable is replaced with real data.

2 variables are available in the variables category **Monitored variables** if there is a limit value violation. When the notification is sent, the variables are replaced by the following data: name of operating procedure, name of sample, name and ID of subsample, value of monitored results, monitoring status, Windows Client.

- '**CurrentMonitoredResult**': This variable supplies information on the result currently being monitored. It can be used only in an optional run **Execute on limit**.
- '**AllMonitoredResults**': This variable provides information on all monitored results of an operating procedure.

See also

Command – Properties (chapter 5.11.8.1, page 431)

IF – Parameters (chapter 5.11.8.70, page 782)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Recording the result monitoring (chapter 5.11.1.11.1, page 408)

Result monitoring – Definition (chapter 5.11.1.11, page 408)

Run in case of a limit value violation – Definition (chapter 5.11.7, page 429)

Setting up notifications (chapter 5.15.1, page 1199)

Text editor – Brief description (chapter 5.11.10, page 849)

5.11.8.73 READ – Parameters

The **READ** command is used to read data from an external instrument that is connected via an RS-232 interface.

The determination can be held during the execution of a **READ** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select

Hold determination. A held subsample can be continued or canceled over the status menu.

The predefined waiting time is stopped when a **READ** command is held. Once the **READ** command is continued, the waiting time continues to run again.

The **READ** command is executed with the following parameters:

Function mode	Select the function mode for reading data: ▪ **Read character string**: The character string sent by the instrument is read and saved in the '**Value**.*Command name*' variables. ▪ **Wait for character string**: The system waits until the character string defined in the **Expected character string** parameter is sent by the instrument.
Instruction	Instruction sent to the instrument before reading via the RS-232 interface.
Expected character string	If **Wait for character string** was selected, then the characters sent via the RS-232 interface are read until the characters match the expected character string and the terminator (known from the specific data of the instrument). Then, the **READ** command is ended and the next command is processed.
Maximum waiting time	The determination of a subsample is canceled with an error if no data from the instrument is received within the maximum waiting time.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

READ – Command variables (chapter 5.11.8.73.1, page 789)

TARE – Parameters (chapter 5.11.8.82, page 803)

WEIGH – Parameters (chapter 5.11.8.85, page 808)

WRITE – Parameters (chapter 5.11.8.86, page 809)

5.11.8.73.1 READ – Command variables

The following variable is created in the process sequence by the **READ** command and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variable available is stored in the **Command variables** variable category.

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**Value**.*Command name*'

Character string (unparsed) that is sent over the RS-232 interface by an external device.

Unit: None

See also

READ – Parameters (chapter 5.11.8.73, page 788)

5.11.8.74 REMOTE IN – Properties

The **REMOTE IN** command is used for scanning remote input lines.

With a remote cable, various instruments can be connected to the **Remote Box MSB** device and their status can be scanned via the remote input lines.

For example, the **849 Level Control** can be connected to the remote connector as additional equipment to the sample changers (Sample Processor) to monitor the fill level in containers for rinsing and waste. Once the **849 Level Control** is connected to the **Remote Box MSB** via the remote cable, the input lines (8 in total) can be scanned in a method run with the **REMOTE IN** command by using a bit pattern. The method run is stopped until the 8-digit bit pattern matches the status of the input lines or until the maximum waiting time has expired. The method run is only continued with the next command once the input signal and the bit pattern match.

Further information on the **Remote Box MSB** and the **849 Level Control** is available on *http://www.metrohm.com*.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*.

In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **REMOTE IN** command:

Parameters

Input signal	Selection of a predefined input signal that scans the status of the sensor connector 1 or 2 of the **849 Level Control**. The sensors can detect both high liquid levels (e.g. warning of overflow of a waste container) as well as low liquid levels (e.g. a supply container running empty). The following predefined input signals are available for scanning the **849 Level Control**: ▪ Sensor **849 - Overall status ok**: No sensor signal active. Bit pattern of the input signal: *****0** ▪ Sensor **849 - Overall status active**: At least 1 sensor signal active. Bit pattern of the input signal: *****1** ▪ Sensor **849 - Full level 1 ok**: Overflow monitoring at sensor 1 ok. Bit pattern of the input signal: ***0**** ▪ Sensor **849 - Full level 1 active**: Overflow warning at sensor 1. The canister is full. Bit pattern of the input signal: ***1**** ▪ Sensor **849 - Full level 2 ok**: Overflow monitoring at sensor 2 ok. Bit pattern of the input signal: **0***** ▪ Sensor **849 - Full level 2 active**: Overflow warning at sensor 2. The canister is full. Bit pattern of the input signal: **1***** ▪ Sensor **849 - Empty level 1 ok**: Empty level monitoring at sensor 1 ok. Bit pattern of the input signal: *0****** ▪ Sensor **849 - Empty level 1 active**: Empty level warning at sensor 1. The canister is empty. Bit pattern of the input signal: *1****** ▪ Sensor **849 - Empty level 2 ok**: Empty level monitoring at sensor 2 ok. Bit pattern of the input signal: 0******* ▪ Sensor **849 - Empty level 2 active**: Empty level warning at sensor 2. The canister is empty. Bit pattern of the input signal: 1******* To scan the remote input signals of other instruments, a user-defined bit pattern can be entered manually with **Enter bit pattern**. If **Enter bit pattern** is selected, the following specific parameter appears: ▪ **Bit pattern**
Bit pattern	Entry of a user-defined bit pattern for the input signal. The bit pattern must contain 8 characters in total. The following characters may be used: ▪ **1** = Input line active ▪ **0** = Input line inactive ▪ ***** = Any status of the input line
Maximum waiting time	Maximum waiting time for receiving input signals. The method run is continued once the requested input signal has been received or the maximum waiting time has expired.

Execute with

In order for a **REMOTE IN** command to be executed, a functional unit of the **Remote Box MSB** type needs to be assigned to the command.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Remote Box MSB – Properties (chapter 5.12.3.29, page 968)

5.11.8.75 REMOTE OUT – Properties

The **REMOTE OUT** command is used for setting remote output lines.

With a remote cable, various instruments can be connected to the **Remote Box MSB** device and their status can be scanned via the remote output lines.

For example, the **843 Pump Station** can be connected to the remote connector as additional equipment to the sample changers (Sample Processor). Both pumps are controlled via remote signals. Once the **843 Pump Station** is connected to the Remote Box via the remote cable, the output lines (14 in total) can be set in a method run with the **REMOTE OUT** command by using a bit pattern.

Further information on the **Remote Box MSB** and the **843 Pump Station** is available on *http://www.metrohm.com*.

Clicking on under **Processes** ▶ **Method** ▶ **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **REMOTE OUT** command:

Parameters

Output signal	Selection of a predefined output signal for the control of the pumps 1 and 2 of the **843 Pump Station**. The pumps can be used for sample preparation or for cleaning vessels. The following predefined output signals for controlling the **843 Pump Station** are available: ▪ Instrument **843 - Pump 1 on**: Start of pump 1. Bit pattern of the output signal: ****1********* ▪ Instrument **843 - Pump 1 off**: Stop of pump 1. Bit pattern of the output signal: ****0********* ▪ Instrument **843 - Pump 2 on**: Start of pump 2. Bit pattern of the output signal: ***1********** ▪ Instrument **843 - Pump 2 off**: Stop of pump 2. Bit pattern of the output signal: ***0********** For controlling other instruments, a user-defined bit pattern can be entered manually under **Enter bit pattern**. If **Enter bit pattern** is selected, the following specific parameter appears: ▪ **Bit pattern**
Bit pattern	Entry of a user-defined bit pattern for the output signal. The bit pattern must contain 14 characters in total. The following characters may be used: ▪ **1** = Output line active ▪ **0** = Output line inactive ▪ ***** = Any status of the output line ▪ **p** = Set a pulse with a pulse duration of 200 ms

Execute with

In order for a **REMOTE OUT** command to be executed, a functional unit of the **Remote Box MSB** type needs to be assigned to the command.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Remote Box MSB – Properties (chapter 5.12.3.29, page 968)

5.11.8.76 REPORT – Parameters

The **REPORT** command is used to create a report as a PDF file or to print it directly on a printer.

In order for all the relevant data to be included in the report by the **REPORT** command, it should be added to the method at the end. Pay particular attention that the **CAL WRITE** command or the **TITER WRITE** command is carried out **before** the **REPORT** command. Otherwise the data is not included in the report.

The **REPORT** command is executed with the parameters listed in the following:

Report template	Selection of a template for the report: ▪ Report templates for sample data ▪ Report templates for subsample data
Output language	Language in which the report is output.
Output format	Selection of the format in which the report is output. ▪ **PDF file** Select the **Target folder** and enter the **PDF file name**. The report is saved as a **PDF file**. ▪ **Paper printout** The report is printed as a **Paper printout** on a printer.
Target folder	Folder in which the report is saved as a PDF file. The following options are available: ▪ Select a target folder by clicking on . ▪ Enter the absolute path (e.g. **C:\Users\Public\Documents\OMNIS\...**). An existing target folder can be supplemented with a new subfolder. This is created by the OMNIS Software.
PDF file name	File name under which the PDF file is saved. The following options are available: ▪ Enter the text; the following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9 ▪ Enter the file name using the formula editor and variable.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

General settings – Subsection (chapter 5.15.3, page 1203)

Operating procedure – Properties (chapter 5.11.1.2, page 383)

5.11.8.77 REQUEST – Parameters

The **REQUEST** command is used to request subsample data or variables during determination.

The determination can be paused manually during the execution of a **REQUEST** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or canceled via the status menu.

After selecting the **REQUEST** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. The following functions and information are available for the **REQUEST** command in the **Parameters** subsection:

General settings	
Display pop-up window	When enabling the **Display pop-up window** check box, the window for the data request will be displayed in the foreground of the sample list. Click on **[Continue]** or use the key combination **[CTRL]**+**[Enter]** to complete the command. If the **Close pop-up window automatically** check box is activated in the window for the data request, then the request is automatically closed as soon as an external instrument (e.g. a balance) receives the CR/LF character string.
Maximum waiting time	Maximum waiting time for entering data. The determination is continued with the next command as soon as the defined waiting time has expired or the command is ended by a user action. With **Unlimited**, the command can be ended only by a user action. Whether the maximum waiting time has been reached is output in the '**TimeoutReached**.Command name' variable. *(see "REQUEST – Command variables", chapter 5.11.8.77.1, page 798)*
Content of the request	
Edit message	Open the window for creating and editing the message that is displayed under **Samples** ▶ **Sample lists** ▶ **Curves and data** ▶ **Live data** or in the pop-up window during the determination.
Define variables	Open the window for defining input fields that are displayed under **Samples** ▶ **Sample lists** ▶ **Curves and data** ▶ **Live data** or in the pop-up window during the determination: *Additional information* For each input field, a variable is selected or defined in which the entered data is saved.
Request buttons	

Buttons	Select the buttons that are displayed when the data is requested. ▪ **Next**: The **[Next]** button is displayed in the request. Clicking on the button continues the determination with the next command. ▪ **User-defined buttons**: The names of 2 buttons can be defined. When the user-defined buttons are used, the '**UserDefinedButton**.Command name' variable outputs the button that was clicked during the request. If **User-defined buttons** is selected, then the following specific parameters appear: – **Highlighted button (output 1)** – **Gray button (output 2)** **Note:** If the corresponding user rights are enabled, then the **[Skip]** button is displayed in addition to the buttons displayed here. Clicking on the button ends the currently running command and continues the determination with the next command.
Highlighted button (output 1)	Enter the name that will be displayed on the highlighted button when the data is requested. Select a name that describes the action that is executed by clicking on the button, e.g. "Rinse system". The highlighted button is preselected by default when the request is displayed. By clicking on the button, the '**UserDefinedButton**.Command name' variable outputs the value 1 and the pop-up window is closed. The variable can, for example, be used in a **IF** command to trigger a specific sequence.
Gray button (output 2) (optional)	Enter the name that will be displayed on the gray button when the data is requested. Select a name that describes the action that is executed by clicking on the button, e.g. "Stop system". By clicking on the button, the '**UserDefinedButton**.Command name' variable outputs the value 2 and the pop-up window is closed. The variable can, for example, be used in a **IF** command to trigger a specific sequence. **Note:** The gray button is optional. If the input field remains empty, then the gray button is not displayed in the request.

Define variables

The following functions and information are available in the **Define variables** window. Additional information on the icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

Name	Designation of the input field. The input field is displayed under **Samples** ▶ **Sample lists** ▶ **Curves and data** ▶ **Live data**.

Save entry in	Selection of the variable in which the data requested during the runtime is saved: ▪ **Variable**: The data requested during the runtime is saved in the selected, existing variable. If **Variable** is selected, then the following specific parameters appear: – **Use as** – **Save input in variable** – **Edit unit** – **Force entry** ▪ **User-defined variable**: The data requested during the runtime is saved in the user-defined variable. Afterwards, this variable is available in the variable selection as a command variable for the **REQUEST** command. If **User-defined variable** is selected, then the following specific parameters appear: – **Use as** – **Variable name** – **Default value** – **Minimum value** – **Maximum value** – **Edit unit** – **Default unit** – **Allow empty field** – **Force entry**
Use as	The following options are available for selection: ▪ **Input field:** The data can be changed manually. ▪ **Sample size:** Weight and unit of weighing data can be applied directly in the **REQUEST** command and can be changed manually after data transmission.
Save input in variable	Selection of an existing variable in which the data requested during the runtime is saved. Clicking (x) opens a dialog in which the desired variable can be selected from the following variable categories: ▪ **Sample data**: Selection of the sample data defined in the sample profile. ▪ **Subsample data**: Selection of the subsample data defined in the operating procedure. ▪ **Method variables**: Selection of the method variables defined in the method. ▪ **System variables**: Selection of the system variables defined in the sample area.
Edit unit	Enable this check box if the unit for the variable is edited during the determination.
Variable name	Name of the user-defined variable. The variable is generated while the command is being executed and is available in the formula editor as a command variable under this variable name.
Default value	Value which is in the input field for the variable as a guideline.

Minimum value	Minimum permitted value for the variable.
Maximum value	Maximum permitted value for the variable.
Default unit	A default unit can be specified for the unit of the variable. If the **Edit unit** check box is enabled, the unit for the variable can be edited.
Allow empty field	Enable the check box if a field without the entry of a value is to be permissible.
Force entry	Enable the check box if the entry of a value is to be forced for empty fields during the determination in the pop-up window of the **REQUEST** command. This option is visible for user-defined variables only if **Allow empty field** has been enabled.

Additional information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

CALC – Parameters (chapter 5.11.8.64, page 768)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Input field – Brief description (chapter 5.11.9.1, page 826)

READ – Parameters (chapter 5.11.8.73, page 788)

REQUEST – Command variables (chapter 5.11.8.77.1, page 798)

Recording weighing data (chapter 5.10.7.4, page 280)

TARE – Parameters (chapter 5.11.8.82, page 803)

Text editor – Brief description (chapter 5.11.10, page 849)

WEIGH – Parameters (chapter 5.11.8.85, page 808)

WRITE – Parameters (chapter 5.11.8.86, page 809)

5.11.8.77.1 REQUEST – Command variables

The following variables are generated by the **REQUEST** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variable available is stored in the **Command variables** variable category.

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**TimeoutReached**.*Command name*'

Status of the maximum waiting time.

- **0**: The maximum waiting time was not reached, e.g. by the user exiting the command or due to an error.
- **1**: The maximum waiting time has been reached.

'**UserDefinedButton**.*Command name*'

If user-defined buttons were selected for the request, then the variable outputs which button was clicked in the process sequence.

- **1**: The highlighted button was clicked during the request.
- **2**: The gray button was clicked during the request.

'**User-defined variable name**.*Command name*'

Value of the **user-defined variable** that has been entered for the **REQUEST** command in the process sequence.

Edit unit can be set.

See also

REQUEST – Parameters (chapter 5.11.8.77, page 794)

5.11.8.78 SEQUENCE – Executing a sequence

The **SEQUENCE** command is used to group commands and methods together into a subordinated run sequence. This run sequence is executed completely before the next command in the method or operating procedure is processed.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

SEQUENCE – Concept (chapter 5.11.8.78.1, page 800)

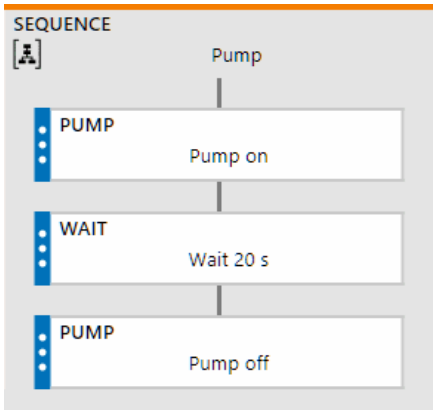
5.11.8.78.1 SEQUENCE – Concept

Structure

With the **SEQUENCE** command, a subordinate run sequence can be defined for commands and methods.

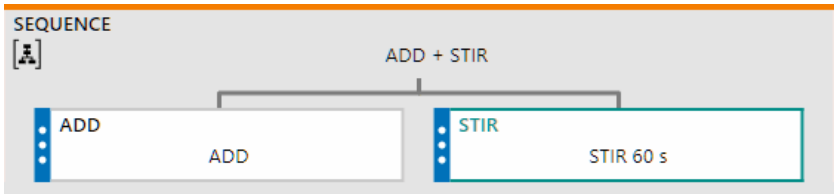
In these run sequences, serial and parallel process sequences are displayed as follows:

- **Serial sequence**



The commands within the run sequence are executed consecutively. The run sequence is concluded as soon as the last command has been completed.

- **Parallel sequence**



The commands within the run sequence are executed in parallel. The run sequence is concluded as soon as the last command has been completed. This makes it possible to synchronize parallel sequences within methods or operating procedures.

Representation in operating procedures and methods

Clicking on ❯ shows the sequence with its commands and methods in a separate area. Clicking ❮ closes the separate area again. The icon next to the arrow indicates the following:

The sequence does not contain any commands.

The sequence contains commands.

See also

Creating and editing a method (chapter 5.11.3.3, page 418)

SEQUENCE – Executing a sequence (chapter 5.11.8.78, page 799)

5.11.8.79 SKIP – Parameters

The **SKIP** command is used to stop a selected command automatically. The **SKIP** command can end commands within the same operating procedure.

If the selected command only starts after the **SKIP** command, an error message appears during the determination. The **SKIP** command should be inserted in the method either after or in parallel to the selected command.

If the results of a selected command are used by a **CALC** command, for example, the calculations may be incomplete.

The **SKIP** command is executed with the parameters listed in the following:

[Select command]	The selected command is stopped during the run sequence of the operating procedure or one of its methods. After the selected command has been stopped, the run is continued with the execution of the next command.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Displaying live data and controlling the run (chapter 5.10.10, page 316)

5.11.8.80 STOP – Parameters

The **STOP** command is used to stop one or more determinations.

If the data permissions are enabled, then only those subsamples are stopped which are visible to the user who starts the determination of the subsample with the **STOP** command.

After selecting the **STOP** command, clicking on opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *(see "Command – Properties", chapter 5.11.8.1, page 431)*. The following functions and information are available for the **STOP** command in the **Parameters** subsection:

Stop subsamples	Select the type of subsamples to be stopped. ▪ **Current**: Only the subsample for which this command is executed is stopped. If a series determination is executed, then determination of the next subsample is started. ▪ **All**: All subsamples are stopped. ▪ **With the same operating procedure**: All subsamples that use the same operating procedure as the subsample for which this command is executed are stopped. The operating procedure must have the same object ID and the same version. ▪ **With the same functional unit with error**: If an error has occurred in a functional unit, then all subsamples that use this functional unit are stopped. If **All**, **With the same operating procedure** or **With the same functional unit with error** is selected, then the following specific parameters will appear: – **Included in** – **With the subsample status**
Included in	Select whether the subsamples are stopped only in the current sample list or in all sample lists. ▪ **Current sample list**: The only subsamples which are stopped are those which are contained in the same sample list as the subsample for which this command is executed. ▪ **All sample lists**: The subsamples in all sample lists are stopped. **Note:** In the **OMNIS Client/Server system**, only the subsamples in the sample lists on the current OMNIS Client are stopped.
With the subsample status	Select whether only the subsamples currently running or all subsamples in a sample series are stopped. ▪ **All**: All subsamples that are currently being executed or are waiting to be executed in a sample series are stopped. ▪ **Waiting for execution**: The subsamples waiting to be executed in a sample series are stopped. The determination of the subsamples currently running is executed to the end.

Additional information on the parameters (e.g., input range, unit, default value) can be found in the tooltips.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

5.11.8.81 SYNC – Parameters

The **SYNC** command is used to synchronize parallel runs within a method.

The **SYNC** command is executed with the following parameters:

Condition	Condition to continue the method. If the condition is fulfilled, the **SYNC** command is ended and the method is continued. Clicking on f_x opens the formula editor, which can be used to define or edit the condition.
[Edit message]	Open the text editor for creating and editing the message. While the determination is being executed, the message is shown in **Samples** ▶ **Sample lists** ▶ **Curves and data** ▶ **Live data**.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

5.11.8.82 TARE – Parameters

The **TARE** command is used to tare a balance. The balance must be connected to the computer on which the OMNIS Software is running.

The **TARE** command is executed with the following parameters:

Waiting time	Time that has to be waited for after having sent the tare command to the balance before the sequence is carried out.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

READ – Parameters (chapter 5.11.8.73, page 788)

WEIGH – Parameters (chapter 5.11.8.85, page 808)

WRITE – Parameters (chapter 5.11.8.86, page 809)

5.11.8.83 TITER WRITE – Parameters

The result of the titer determination of a connected solution can be saved to the settings of the bottle cap used with the **TITER WRITE** command. The titer is the correction factor that indicates the deviation of the actual concentration of a titrant from the nominal concentration. It is specific to the respective titrant and is determined from the mean values of all sub-samples of a sample.

When the titer is saved, the sample ID, the titer, the titer unit, the number of subsamples, the standard deviation of the titer as well as time and date of the titer determination are saved in the memory location.

Depending on the combination of instruments used, the titer data is saved to the following memory locations:

- **Dosing Drive** with connected **Cylinder Unit**: The titer data is saved to the RFID tag of the bottle cap.
- **800 Dosino** with connected **807 Dosing Unit**: The titer data is saved to the memory chip of the **807 Dosing Unit**.
- **805 Dosimat** with connected **806 Exchange Unit**: The titer data is saved to the memory chip of the **806 Exchange Unit**.

For a **TITER WRITE** command to be executed, a work system with one of the following functional units must be assigned to the method that contains the command under **Processes** ▶ **Method** ▶ **Properties** ▶ **Execute with**:

- **Dosing Drive** with connected **Cylinder Unit**
- **800 Dosino** with connected **807 Dosing Unit**
- **805 Dosimat** with connected **806 Exchange Unit**

The required solution must be connected to this.

For the data of the titer determination to be written correctly, the following conditions must also be fulfilled in the run:

- A titration command (**DET**, **MET**, **SET**, **TET**, **KFT**) and then a calculation command (**CALC**) must first be executed in the method.
- Only after these commands, a **TITER WRITE** command can be executed for which the titration command and the calculation command are referenced in the parameters.
- The **TITER WRITE** command must be executed **prior** to the **REPORT** command if a report is to be created in the method. Otherwise the data is not included in the report.

The **TITER WRITE** command is executed with the parameters listed in the following:

Name of the titration command	Selection of the titration command that was run for the titer determination. All titration commands that were executed in the same method **before** the **TITER WRITE** command can be selected. The name of the titration command has to be unique and must not be used multiple times in the method.
Name of the calculation command	Selection of the calculation command that leads to the results of the titer determination. This includes the mean value, the decimal places, the standard deviation, the number of subsamples and the titer unit. All calculation commands that were executed in the same method **before** the **TITER WRITE** command can be selected. The name of the required calculation command has to be unique and must not be used multiple times in the method. In order to write the mean value, the number of subsamples and the standard deviation of the titer, the function **Calculate statistics** has to be activated in the selected calculation command beforehand.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Saving titer (chapter 5.11.8.83.1, page 805)

5.11.8.83.1 Saving titer

The titer of a connected solution can be determined and the result can be saved on the writable RFID tag in the memory chip of the bottle cap used with the **CALC** and **TITER WRITE** commands.

Prerequisites:

- A work system with a functional unit of the **Dosing Unit** type must be assigned to the method.
- A **Liquid Adapter** with a **Solution with bottle cap single-use** or a **Solution with bottle cap multi-use** must be connected to this functional unit.

1 Creating a method

- Create or select a method in **Processes** ▶ **Methods**.

The method is opened.

2 Inserting commands

- Insert the following commands in the method in the correct sequence.
  - A titration command (**DET**, **SET**, **MET**, **KFT**). It needs to have a unique name in the method as it is referenced later on.
  - A calculation command (**CALC**). It needs to have a unique name in the method as it is referenced later on.
    In order to write the mean value, the number of subsamples and the standard deviation of the titer, the **Calculate statistics** function must be activated in the calculation command.
  - A **TITER WRITE** type command
  - A **REPORT** type command if a report is to be created in the method.

The method contains all the necessary commands in the correct sequence.

3 Parameterizing TITER WRITE

- Open the parameters of the **TITER WRITE** command.
- Open the selection list in **Name of the titration command** and select the desired command.
- Open the selection list in **Name of the calculation command** and select the desired command.

The **TITER WRITE** command is linked to the titration command and the calculation command.

4 Carrying out the determination

- Carry out the titer determination with the connected solution.

The result of the titer determination is saved on the bottle cap. The sample ID, the titer, the titer unit, time and date of the titer determination are saved, as well as the mean value, the number of subsamples and the standard deviation if statistics calculation is activated.

The result needs to be monitored as a variable in order to prevent invalid values from the titer determination from being saved. This can be defined in **Processes** ▶ **Operating procedure** ▶ **Properties** ▶ **Result monitoring**.
(see "Recording the result monitoring", chapter 5.11.1.11.1, page 408)

See also

Recording the result monitoring (chapter 5.11.1.11.1, page 408)

TITER WRITE – Parameters (chapter 5.11.8.83, page 804)

TITER WRITE – Parameters (chapter 5.11.8.83, page 804)

5.11.8.84 WAIT – Parameters

The **WAIT** command is used to interrupt the process sequence for a defined time period or until a message is confirmed by the user. The determination can be held manually during the execution of a **WAIT** command with waiting time. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**.

The predefined waiting time is stopped when a **WAIT** command is held manually. Once the **WAIT** command is continued, the waiting time continues to run again.

The **WAIT** command is executed with the following parameters:

Wait for user action	Wait until the user confirms the message displayed in **Samples** ▶ **Sample lists** ▶ **Curves and data** ▶ **Live data** by clicking **[Continue]**.
Predefined waiting time	Wait until the time defined in the parameter **Waiting time** has expired. If **Predefined waiting time** is selected, the following specific parameter is displayed: ▪ **Waiting time**
Waiting time	Waiting time after which the process sequence is continued.
[Edit message]	Open the text editor for creating and editing the message that is displayed during the determination under **Samples** ▶ **Sample lists** ▶ **Curves and data** ▶ **Live data**.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Command – Properties (chapter 5.11.8.1, page 431)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Text editor – Brief description (chapter 5.11.10, page 849)

5.11.8.85 WEIGH – Parameters

The **WEIGH** command is used to request the weighing result of a balance. The balance must be connected to the computer on which the OMNIS Software is running.

The **WEIGH** command is executed with the following parameters:

Maximum waiting time	Maximum waiting time after which the determination is canceled because no data could be received from the balance.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

READ – Parameters (chapter 5.11.8.73, page 788)

TARE – Parameters (chapter 5.11.8.82, page 803)

WEIGH – Command variables (chapter 5.11.8.85.1, page 808)

WRITE – Parameters (chapter 5.11.8.86, page 809)

5.11.8.85.1 WEIGH – Command variables

The following variables are generated by the **WEIGH** command during the process sequence and can be used in a formula under the '**Variable name**.*Command name*' designation.

The variables available are stored in the **Command variables** variable category.

'**Finished**.*Command name*'

Status of the command.

- **Invalid**: The command has not been started (yet).
- **0**: The command is still running.
- **1**: The command has been completed correctly.
- **2**: The command has not been completed correctly. An error or a warning occurred.
- **3**: The command was skipped either by a **SKIP** command or manually in the **Live data**.
- **4**: The command was stopped either with a manual action by the user (stop or emergency stop), by a **STOP** command or because of an error in a command that is running in parallel.

'**Weigh.Result**.*Command name*' Numerical value of the weighing result. Unit: defined in the '**Unit.Result**.*Command name*' variable
'**Unit.Result**.*Command name*' Unit of the weighing result.

See also

WEIGH – Parameters (chapter 5.11.8.85, page 808)

5.11.8.86 WRITE – Parameters

The **WRITE** command is used to send data to an external device that is connected via an RS-232 interface.

The determination can be paused manually during the execution of a **WRITE** command. To do so, open the status menu by clicking with the right or left mouse button on the status display of the running subsample and select **Hold determination**. A held subsample can be continued or stopped over the status menu.

The **WRITE** command is executed with the parameters listed in the following:

Character string	Character string that is sent to the external instrument via the RS-232 interface. A maximum of 1,000 characters can be entered. ***NOTICE:*** When **Formula** is selected, the function **NumberToText** must precede it or a variable of the type **Text** must be selected. A variable from one of the variables categories **Sample data**, **Subsample data**, **Method variables** or **System variables** for which the type **Text** was defined during its creation can be selected for this purpose.

Further information on the parameters (e.g. input range, unit, default value) can be found in the tooltips.

See also

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing a method (chapter 5.11.3.3, page 418)

READ – Parameters (chapter 5.11.8.73, page 788)

TARE – Parameters (chapter 5.11.8.82, page 803)

WEIGH – Parameters (chapter 5.11.8.85, page 808)

5.11.8.87 Command – Directory

- *Automation commands*
- *Dosing commands*
- *Calibration commands*
- *Measuring commands*
- *Spectroscopy commands*
- *Titration commands*
- *Conditioning commands*
- *Additional commands*

Automation command	Functional unit	Instrument
CLOSE GRIPPER	Main Module Pick&Place	OMNIS Sample Robot
	OMNIS Main Module	OMNIS Sample Robot, OMNIS Sample Robot NIR, OMNIS Sample Robot Oven
FLOW	Gas Flow Unit	OMNIS Sample Robot Oven, 874 Oven Sample Processor
INIT MAIN MODULE	Tower	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler, 874 Oven Sample Processor
LIFT	Main Module Pick&Place, Pick&Place Module	OMNIS Sample Robot
	OMNIS Main Module	OMNIS Sample Robot, OMNIS Sample Robot NIR, OMNIS Sample Robot Oven
	Oven Module	OMNIS Sample Robot Oven
	Tower	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler, 874 Oven Sample Processor
MOVE TO EXT	Tower	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler
MOVE TO RACK	Main Module Pick&Place	OMNIS Sample Robot
	OMNIS Main Module	OMNIS Sample Robot, OMNIS Sample Robot NIR, OMNIS Sample Robot Oven
	Tower	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler, 874 Oven Sample Processor
MOVE TO WORKSTATION	Main Module Pick&Place, Pick&Place Module	OMNIS Sample Robot
	OMNIS Main Module, Liquid Sample Presentation, Solid Sample Presentation, Oven Module	OMNIS Sample Robot, OMNIS Sample Robot NIR, OMNIS Sample Robot Oven

Automation command	Functional unit	Instrument
OPEN GRIPPER	Main Module Pick&Place	OMNIS Sample Robot
	OMNIS Main Module	OMNIS Sample Robot, OMNIS Sample Robot NIR, OMNIS Sample Robot Oven
PARK LID	Main Module Pick&Place, OMNIS Main Module	OMNIS Sample Robot
PREP SPEC	Liquid Sample Presentation	OMNIS NIR Analyzer Liquid, OMNIS NIR Analyzer Liquid/Solid
PUMP	Pump Module	OMNIS Sample Robot
	Membrane Pump (Rinse), Membrane Pump (Aspirate), External Pump Socket	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler
RETRIEVE LID	Main Module Pick&Place, Pick&Place Module, OMNIS Main Module	OMNIS Sample Robot
ROTATE	Oven Module	OMNIS Sample Robot Oven
ROTATE ANGLE	Tower	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler
SLIDE	Pick&Place Module	OMNIS Sample Robot
STIR	OMNIS Rod Stirrer, Magnetic Stirrer	OMNIS Coulometer, OMNIS Coulometer Module, OMNIS Dosing Module, OMNIS Sample Robot, OMNIS Sample Robot Oven, OMNIS Titrator, OMNIS Titration Module
	801 Stirrer, 803 Ti Stand, 804 Ti Stand	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Tower Stirrer Socket	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler
SWING ANGLE	Tower	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler
TEMP	Oven Unit	OMNIS Sample Robot Oven, 874 Oven Sample Processor
TRANSPORT OVEN VIAL	Oven Module	OMNIS Sample Robot Oven
VESSEL REMOVAL	Liquid Sample Presentation	OMNIS NIR Analyzer Liquid, OMNIS NIR Analyzer Liquid/Solid

Dosing command	Functional unit	Instrument
ADD	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	800 Dosino	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 890 Titrando, 904 Titrando, 906 Titrando
ASPIRATE	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	800 Dosino	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 907 Titrando
COMPENSATE	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	800 Dosino	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 907 Titrando

Dosing command	Functional unit	Instrument
DOSE	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	800 Dosino	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 907 Titrando
FILL	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	800 Dosino	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 890 Titrando, 904 Titrando, 906 Titrando
PISTON END	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	800 Dosino	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando

Dosing command	Functional unit	Instrument
PISTON POS	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	800 Dosino	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
SOLVENT HANDLING	OMNIS Solvent Module	OMNIS Solvent Module
VALVE POS	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	800 Dosino	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando

Calibration command	Functional unit	Instrument
CAL CONC	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Analog	855 Robotic Titrosampler, 867 pH Module, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
CAL COND	Measuring Module Conductivity	OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Conductivity	856 Conductivity Module
CAL pH	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Measuring Interface iConnect	867 pH Module, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 867 pH Module, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
CAL WL	2060 The NIR, Liquid Sample Presentation, Solid Sample Presentation	2060 The NIR, OMNIS NIR Analyzer Liquid, OMNIS NIR Analyzer Liquid/Solid, OMNIS NIR Analyzer Solid

Calibration command	Functional unit	Instrument
REF STD	2060 The NIR	2060 The NIR
VAL REF STD	2060 The NIR	2060 The NIR
VAL WL	2060 The NIR, Liquid Sample Presentation, Solid Sample Presentation	2060 The NIR, OMNIS NIR Analyzer Liquid, OMNIS NIR Analyzer Liquid/Solid, OMNIS NIR Analyzer Solid

Measuring command	Functional unit	Instrument
MEAS CONC	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Analog	855 Robotic Titrosampler, 867 pH Module, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
MEAS COND	Measuring Module Conductivity	OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Conductivity	856 Conductivity Module
MEAS Ipol	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Coulometry	OMNIS Coulometer, OMNIS Coulometer Module
	Measuring Interface Analog	852 Titrando, 855 Robotic Titrosampler, 867 pH Module, 888 Titrando, 890 Titrando, 901 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Interface Coulometry	851 Titrando, 852 Titrando
MEAS pH	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Measuring Interface iConnect	867 pH Module, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 867 pH Module, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
MEAS REF SPEC	2060 The NIR, Liquid Sample Presentation, Solid Sample Presentation	2060 The NIR, OMNIS NIR Analyzer Liquid, OMNIS NIR Analyzer Liquid/Solid, OMNIS NIR Analyzer Solid
MEAS SPEC	2060 The NIR, Liquid Sample Presentation, Solid Sample Presentation	2060 The NIR, OMNIS NIR Analyzer Liquid, OMNIS NIR Analyzer Liquid/Solid, OMNIS NIR Analyzer Solid

Measuring command	Functional unit	Instrument
MEAS T	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Coulometry	OMNIS Coulometer, OMNIS Coulometer Module
	Measuring Interface iConnect	867 pH Module, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	852 Titrando, 855 Robotic Titrosampler, 867 pH Module, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Interface Coulometry	851 Titrando, 852 Titrando
MEAS U	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Measuring Interface iConnect	867 pH Module, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 867 pH Module, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando

Spectroscopy command	Functional unit	Instrument
PREDICT	–	–
TEST NOISE	2060 The NIR, Liquid Sample Presentation, Solid Sample Presentation	2060 The NIR, OMNIS NIR Analyzer Liquid, OMNIS NIR Analyzer Liquid/Solid, OMNIS NIR Analyzer Solid
TEST WL	2060 The NIR, Liquid Sample Presentation, Solid Sample Presentation	2060 The NIR, OMNIS NIR Analyzer Liquid, OMNIS NIR Analyzer Liquid/Solid, OMNIS NIR Analyzer Solid

Titration command	Functional unit	Instrument
BRC CC Ipol	Measuring Module Coulometry	OMNIS Coulometer, OMNIS Coulometer Module

Titration command	Functional unit	Instrument
DET Ipol	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Analog	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 904 Titrando, 906 Titrando
DET pH	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface iConnect	888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 904 Titrando, 906 Titrando

Titration command	Functional unit	Instrument
DET U	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface iConnect	888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 904 Titrando, 906 Titrando
KFC	Measuring Module Coulometry	OMNIS Coulometer, OMNIS Coulometer Module
	Interface Coulometry	851 Titrando, 852 Titrando
KFT Ipol	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Analog	852 Titrando, 888 Titrando, 890 Titrando, 901 Titrando, 906 Titrando, 907 Titrando
	Interface Coulometry	852 Titrando
	800 Dosino	852 Titrando, 888 Titrando, 901 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	852 Titrando, 888 Titrando, 901 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 890 Titrando, 906 Titrando
MET COND	Measuring Module Conductivity	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Conductivity	856 Conductivity Module
	800 Dosino	856 Conductivity Module
	805 Dosimat	856 Conductivity Module

Titration command	Functional unit	Instrument
MET Ipol	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Analog	852 Titrando, 855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	852 Titrando, 855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	852 Titrando, 855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 904 Titrando, 906 Titrando
MET pH	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface iConnect	888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 904 Titrando, 906 Titrando

Titration command	Functional unit	Instrument
MET U	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface iConnect	888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 888 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 904 Titrando, 906 Titrando
SET Ipol	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Analog	852 Titrando, 855 Robotic Titrosampler, 888 Titrando, 901 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Interface Coulometry	852 Titrando
	800 Dosino	852 Titrando, 855 Robotic Titrosampler, 888 Titrando, 901 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	852 Titrando, 855 Robotic Titrosampler, 888 Titrando, 901 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 904 Titrando, 906 Titrando

Titration command	Functional unit	Instrument
SET pH	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface iConnect	888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 904 Titrando, 906 Titrando
SET U	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface iConnect	888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 888 Titrando, 901 Titrando, 902 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	888 Titrando, 904 Titrando, 906 Titrando

Titration command	Functional unit	Instrument
STAT pH	Measuring Interface iConnect	902 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 902 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 902 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 902 Titrando, 906 Titrando, 907 Titrando
STAT U	Measuring Interface iConnect	902 Titrando, 906 Titrando, 907 Titrando
	Measuring Interface Analog	855 Robotic Titrosampler, 902 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 902 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 902 Titrando, 906 Titrando, 907 Titrando
STDADD ISE auto	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Analog	855 Robotic Titrosampler, 867 pH Module, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 867 pH Module, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 867 pH Module, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	904 Titrando, 906 Titrando

Titration command	Functional unit	Instrument
STDADD ISE dos	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Measuring Module Analog	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module
	Measuring Interface Analog	855 Robotic Titrosampler, 867 pH Module, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	800 Dosino	855 Robotic Titrosampler, 867 pH Module, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	805 Dosimat	855 Robotic Titrosampler, 867 pH Module, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Internal Dosing Drive	904 Titrando, 906 Titrando
TET	Measuring Module Digital	OMNIS Titrator, OMNIS Titration Module
	Dosing Drive	OMNIS Dosing Module, OMNIS Titrator, OMNIS Titration Module

Conditioning command	Functional unit	Instrument
COND CHECK	–	–
COND OFF	–	–
COND ON	–	–

Additional commands	Functional unit	Instrument
ADD TO SAMPLE LIST	–	–
CAL WRITE	–	–
CALC	–	–
CALL WEB API	–	–
COLLECT	–	–
CONSUME SUBSAMPLE	–	–
EVAL BASE STATISTICS	–	–
EVAL LINEAR REGRESSION	–	–
EXPORT	–	–

Additional commands	Functional unit	Instrument
IF	–	–
LOOP	–	–
NOTIFY	–	–
READ	Serial Device	–
REMOTE IN	Remote Box MSB	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
REMOTE OUT	Remote Box MSB	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 846 Dosing Interface, 851 Titrando, 852 Titrando, 855 Robotic Titrosampler, 856 Conductivity Module, 867 pH Module, 874 Oven Sample Processor, 888 Titrando, 890 Titrando, 901 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
REPORT	–	–
REQUEST	–	–
SEQUENCE	–	–
SKIP	–	–
STOP	–	–
SYNC	–	–
TARE	Balance, Cubis II Balance	
TITER WRITE	–	–
WAIT	–	–
WEIGH	Balance, Cubis II Balance	
WRITE	Serial Device	–

See also

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Creating a work system (chapter 5.12.4.4, page 989)

Creating and editing a method (chapter 5.11.3.3, page 418)

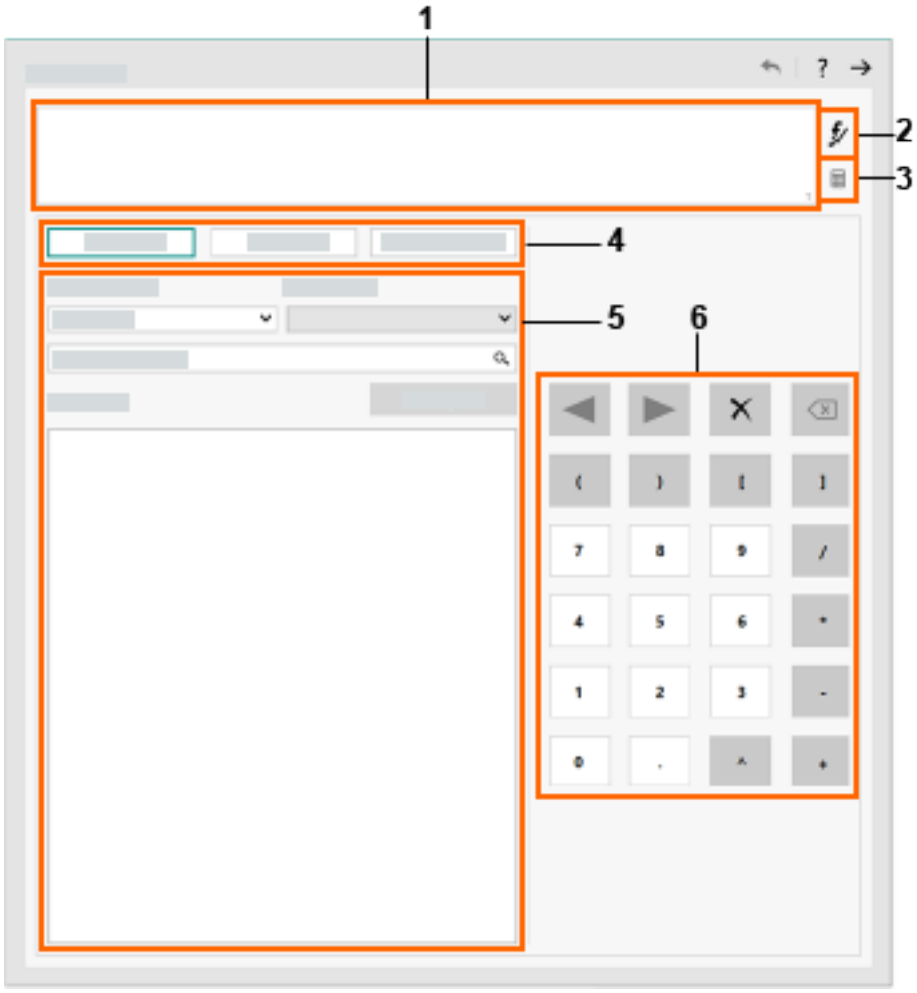
Functional unit – Directory (chapter 5.12.3.1, page 894)

Instruments – Directory (chapter 5.12.2.2, page 854)

5.11.9 Formula editor – Brief description

The formula editor serves as a support when entering formulas for result calculation. It is equipped with a syntax check that is triggered automatically when the formula is applied or that can also be triggered manually.

The general rules of priority apply for the calculation operations defined in the formula. The **Formula editor** dialog window contains the following elements:



1 Input field
Input field for the calculation formula.

2 Syntax check
Check validity of the entered formula.

3 Display result

By clicking on , the formula is calculated and the result is displayed. All variables used must be known and must have a valid value. If the value of a variable used is not generated until the runtime of a determination, then clicking on will display the result **Invalid**. The syntax of the formula must be correct.

4 Buttons

Additional options for entering a formula are displayed with the buttons beneath the input field.

The list of the variables available for the calculation formula is displayed under **[Variables]**. The variables can be filtered in accordance with their function.

The list of the functions that can be used in the formula is displayed under **[Functions]**.

The list with additional operators for linking operands in the formula is displayed in **[Other operators]**.

5 Search result

The selected formula is inserted into the input field by double-clicking on the search result or by clicking on **[Insert]**.

6 Numerical keypad

Buttons for the quick entry of numbers, arithmetic operators and brackets.

See also

Functions – Directory (chapter 5.11.9.5, page 831)

Input field – Brief description (chapter 5.11.9.1, page 826)

Operators – Directory (chapter 5.11.9.4, page 830)

Variables – Directory (chapter 5.11.9.3, page 827)

5.11.9.1 Input field – Brief description

The calculation formula is entered in the input field of the formula editor. The following options are available for the entry:

Entry via keyboard

- **Numbers**
  Numbers as well as mathematical functions can be entered directly via the keyboard.
- **Text**
  Text must be enclosed in quotation marks **"** (e.g. **"my text"**).
- **Variables**
  Variables must be enclosed in apostrophes **'** (e.g., **'Temperature.EP{x}.***Command name***'**).
- **Time**
  Time indications must always be entered using the **Time( )** function.

Entry using the buttons

- Mathematical operators, parentheses or brackets and numbers can be inserted in the formula by clicking the corresponding buttons.

- With the **[Variables]**, **[Functions]** and **[Other operators]** buttons, the variables, functions and operators available for the formula can be displayed. They can be inserted from the list with a double-click or by clicking **[Insert]**.

5.11.9.2 Formula editor – Statistics calculation

The mean value, the absolute and relative standard deviation of results *x* are calculated with the following formulas:

Mean value	$\bar{x} = \frac{1}{n} \cdot \sum_{i=1}^{n} x_i$
Absolute standard deviation	$s_{abs} = \left\| \sqrt{\frac{1}{n-1} \cdot \sum_{i=1}^{n} (x_i - \bar{x})^2} \right\|$
Relative standard deviation in %	$s_{rel} = 100 \cdot \frac{s_{abs}}{\bar{x}}$

The calculation of the mean value and the standard deviation are carried out with the input data (results) with full accuracy. If you do not wish that, round off the input data by using the **Round()** function in the formulas for the results. With this, the input data (results) and the output data (mean value, standard deviation) can be rounded off to the accuracy specified by the user.

5.11.9.3 Variables – Directory

Variables are created automatically by the OMNIS Software with the following actions:

- When recording sample data
- During an ongoing determination
- At the end of a determination

Variables can be selected in the formula editor. The variable values can either be used for further calculations or output as a result in reports or entered as a condition in the **IF** command.

The variables in the formula editor must be inserted again afterwards if methods are renamed that contain variables that were used to define a condition in the **IF** command.

Variable category	Subcategory	Variable type
Sample data	Selection of the sample profile	Variables that are defined in the sample profile as sample data. Syntax: '*Variable name*.**CurrentSampleData**' The *Variable name* corresponds to the name that was defined in the sample profile for the sample data. The following variables are available by default: ▪ Sample name (e.g. for use as the file name of reports and exports): '**Name.CurrentSample**'
Subsample data	Selection of the operating procedure	Variables that are defined in the **Parameters** subsection of the **Properties** window of an operating procedure as subsample data. Syntax: '*Variable name*.**CurrentSubSampleData**' The *variable name* corresponds to the name that was defined in the operating procedure for the subsample data. The following variables are available by default: ▪ User ID of the user that created the subsample: '**CreatedBy.CurrentSubsample**' ▪ Creation date of the subsample: '**CreationTimestamp.CurrentSubsample**' ▪ Determination run (single determination, series determination, parallel determination): '**ExecutionMode.CurrentSubsample**' ▪ Subsample name (e.g. for use as the file name of reports and exports): '**Name.CurrentSubsample**' ▪ User ID of the user that started the determination: '**StartedBy.CurrentSubsample**' ▪ Type of stop via which the determination is canceled. The variable can be used only as a condition in a IF command: '**StopType.CurrentSubsample**' **1**: The determination was automatically stopped, e.g. by a STOP command. **2**: The determination was manually stopped, e.g. by clicking on a button.
Method variables	Selection of the method	Variables that are defined in the **Parameters** subsection of the **Properties** window of a method. Syntax: '*Variable name*.**CurrentMethod**' The *variable name* corresponds to the name that was defined for the method variable. **Note:** The variables in the formula editor must be inserted again afterwards if methods are renamed which contain variables that were used in the **IF** command.

Variable category	Subcategory	Variable type
Command variables	All variables or selection of the command	Variables that are generated by the individual commands in the process sequence. The search result is dependent on the commands used in the method. Syntax: '*Variable name*.*Command name*'
Equipment variables	**Assigned work systems**	Variables that are generated by the individual commands in the process sequence. The selection is dependent on the used functional units of those work systems that are assigned to the method. Syntax: '*Variable name*.*Command name*' Variables with which the first and last use of a work system by a method can be scanned are available by default: ▪ '**FirstUse.CurrentWorkSystem**.*Method name*' ▪ '**LastUse.CurrentWorkSystem**.*Method name*'
Equipment variables	**Sensors**	Variables that are available for the sensors that are connected to the instruments. Syntax: '*Variable name*.*Sensor name*'
Equipment variables	**Racks**	Variables that are available for the sample racks that are placed on top of the sample robot. Syntax: '*Variable name*.*Rack name*'
Equipment variables	**Solutions**	Variables that are available for the solutions that are connected to the instruments. Syntax: '*Variable name*.*Solution name*'
System variables		Variables that are defined across the system. A system variable can be used as text, as value or as its unit in methods and operating procedures. Syntax: '**Value**.*Variable name*.**System**' '**Unit**.*Variable name*.**System**' The *variable name* corresponds to the name that was defined for the system variable.

When using variables, the data type must also be observed (**Number**, **Text** or **Date/Time**).

In the case of variables with index **{x}**, the desired number 1 - 9 must be entered for **x** (e.g., ''**Meas.EP{3}**.*Command name*' for the third endpoint). **x** = 1 is entered in the formula editor as default value.

5.11.9.4 Operators – Directory

Different operator types can be used in the formula editor to carry out calculations with operands or to compare operands.

The **arithmetic operators** for calculations are visible as buttons in the formula editor. A selection of **logical operators** and **comparative operators** can be displayed by clicking on **Other operators**.

Arithmetic operators

The arithmetic operators are visible as buttons in the formula editor and are used to carry out calculations with operands.

+	Addition
-	Subtraction
*	Multiplication
/	Division
^	Potentiation

The operands can be entered either directly or as a variable and must be of the **Number** type.

Logical operators

The logical operators are used to link two operands.

The entries are interpreted as follows:

- All numbers that are not 0 are interpreted as 1 (e.g., 5, 0.04, –8).
- Entries of the **Text** or **Date/Time** types are always interpreted as 1 (e.g., "Hello", "0", Time()).
- The result type is always a number (1 = true, 0 = false).

Logical AND	Both linked expressions must be fulfilled.
Logical OR	At least one of the linked expressions must be fulfilled.

The following cases are possible:

AND	Operand 1	Operand 2	Result
	1	1	1
	0	1	0
	1	0	0
	0	0	0

OR	Operand 1	Operand 2	Result
	1	1	1
	0	1	1
	1	0	1
	0	0	0

The operands can be entered either directly or as a variable and can be of the **Text**, **Number** or **Date/Time** type.

Comparative operators

The comparative operators are used to compare 2 operands.

=	Both operands must have the same value.
>	The first operand must be greater than the second operand.
> =	The first operand must be greater than or equal to the second operand.
<	The first operand must be less than the second operand.
< =	The first operand must be less than or equal to the second operand.
< >	The operands must not have the same value.

Examples:

- 5 > 2 = 1
- 5 < 2 = 0
- 'Temperature.Final.Dynamic pH titration 1.Test method.Operating procedure 1.Subsample 1.Sample 1' > 25 = 1

The operands can be entered either directly or as a variable. They can be of the **Number** or **Date/Time** type. The result type is always a number (1 = true, 0 = false).

5.11.9.5 Functions – Directory

The following functions can be used in the formula editor:

Arithmetic

- **Abs** – Absolute value
  (see "Abs – Absolute value", chapter 5.11.9.5.1, page 833)
- **Ceiling** – Rounding-up function
  (see "Ceiling – Rounding-up function", chapter 5.11.9.5.3, page 834)
- **Exp** – Exponential function
  (see "Exp – Exponential function", chapter 5.11.9.5.6, page 836)

- **Floor** – Rounding-down function
  (see "Floor – Rounding-down function", chapter 5.11.9.5.7, page 836)
- **Ln** – Natural logarithm
  (see "Ln – Natural logarithm", chapter 5.11.9.5.10, page 838)
- **Log** – Common logarithm
  (see "Log – Common logarithm", chapter 5.11.9.5.9, page 837)
- **Pow** – Power
  (see "Pow – Power", chapter 5.11.9.5.14, page 839)
- **Round** – Round
  (see "Round – Rounding", chapter 5.11.9.5.18, page 843)
- **Sign** – Sign function
  (see "Sign – Sign function", chapter 5.11.9.5.19, page 844)
- **Sqrt** – Square root
  (see "Sqrt – Square root", chapter 5.11.9.5.20, page 844)
- **Truncate** – Truncate to integer
  (see "Truncate – Truncate to integer", chapter 5.11.9.5.28, page 849)

Date/Time

- **Time** – Time
  (see "Time – Time", chapter 5.11.9.5.24, page 846)

Type conversion

- **NumberToText** – Convert number to text
  (see "NumberToText – Convert number to text", chapter 5.11.9.5.13, page 839)
- **TextToNumber** – Convert text to number
  (see "TextToNumber – Convert text to number", chapter 5.11.9.5.23, page 846)
- **TimeToNumber** – Convert date/time to number
  (see "TimeToNumber – Convert date/time to number", chapter 5.11.9.5.25, page 847)
- **TimeToText** – Convert date/time to text
  (see "TimeToText – Convert date/time to text", chapter 5.11.9.5.26, page 848)

Text

- **Concat** – Concatenate
  (see "Concat - Concatenating texts", chapter 5.11.9.5.4, page 835)
- **TextPosition** – Return the position of character string searched for
  (see "TextPosition – Return position of character string searched for", chapter 5.11.9.5.22, page 845)
- **Trim** – Remove blank spaces / character string
  (see "Trim – Remove blank spaces / character string", chapter 5.11.9.5.27, page 848)

- **SubText** – Return part of a character string
  (see "SubText – Return part of a character string", chapter 5.11.9.5.21, page 844)
- **SubText** – Return part of a character string
  (see "SubText – Return part of a character string", chapter 5.11.9.5.21, page 844)
- **Replace** – Replace character string
  (see "Replacing – Replace character string", chapter 5.11.9.5.17, page 842)
- **Length** – Length of a character string
  (see "Length – Length of a character string", chapter 5.11.9.5.8, page 837)

Miscellaneous

- **Case** – Condition
  (see "Case – Condition", chapter 5.11.9.5.2, page 834)
- **Error** – Error case
  (see "Error – Error case", chapter 5.11.9.5.5, page 835)
- **Max** – Maximum
  (see "Max – Maximum", chapter 5.11.9.5.11, page 838)
- **Min** – Minimum
  (see "Min – Minimum", chapter 5.11.9.5.12, page 838)
- **Rand** – Generate random number
  (see "Rand – Generate random number", chapter 5.11.9.5.15, page 840)
- **RegEx** – Regular expression
  (see "RegEx – Regular expression", chapter 5.11.9.5.16, page 840)

5.11.9.5.1 Abs – Absolute value

Syntax

y = Abs(number)

Returns the absolute value of the entered number, i.e. the amount of the number.

Parameter

Number

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.

Examples

- Abs(–55.3) = 55.3
- Abs('Temperature.EP{x}.*Command name*') = value of the variable 'Temperature.EP{x}.*Command name*' without algebraic sign.

5.11.9.5.2 Case – Condition

Syntax

- **y = Case(Condition;Value_true;Value_false)**
  Returns **value_true** if the **condition** is true. Otherwise **Value_false** is returned.
- **y = Case(Condition;Value_true;Value_false;Value_error)**
  Returns **value_true** if the **condition** is true. Otherwise **Value_false** is returned. If an error occurs in the condition (result **invalid**), then **value_error** is returned.

Parameters

- **Condition**
  Any variable (**Number** type) can be entered here, or a logic operation can be performed, the operators of which can be transferred either directly or as a variable.
- **Value_true**
  If **Condition = 1** (e.g., 1 < 2), this parameter is saved as a result of the function.
- **Value_false**
  If **Condition <> 0** (e.g., 1 > 2), this parameter is saved as a result of the function.
- **Value_error**
  If **Condition = invalid**, this parameter is saved as a result of the function.
  These parameters for the values can be transferred either directly or as a variable and can be of the **Text**, **Number** or **Date/Time** type. Entire operations can also be transferred here. Parameters in the form of **Text**, must be written in quotation marks.

Example

- Case('CellConstant.CALCOND' < 50; "Expression is TRUE";"Expression is FALSE";"ERROR: Expression could not be evaluated") = If the result is smaller than 50, **Expression is TRUE** will be returned; if it is greater than or equal to 50, **Expression is FALSE** will be returned. If the result could not be calculated, **ERROR: Expression could not be evaluated** will be returned.

5.11.9.5.3 Ceiling – Rounding-up function

Syntax

y = Ceiling(number)

Returns the nearest integer greater than or equal to the entered number.

Parameters

Number

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **invalid** and an error message will appear.

Examples

- Ceiling(2.9) = 3
- Ceiling(1.01) = 2
- Ceiling(3) = 3
- Ceiling(-1.1) = -1
- Ceiling(0) = 0

5.11.9.5.4 Concat - Concatenating texts

Syntax

y = Concat(Text1;Text2; ... ;Textx)

Connects the specified single text parts **Text1** - **Textx** to a new whole text.

Parameter

- **Text1 - Textx**
  The parameter can be indicated either as a variable of the **Text** or of the **Number** type or directly as text. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.
  Variable: Entry with apostrophes '*Variable name*'
  Text: Entry with quotation marks "*Example text*"

Examples

- Concat("Content: ";'MeanValue.Result1.Calc1';" ± ";'StandardDeviation.Result1.Calc1';" mg/L") = Content: 24.58 ± 0.76 mg/L
- Concat("The sample was measured ";'LoopCount.Loop1';" times.") = The sample was measured 4 times.

5.11.9.5.5 Error – Error case

Syntax

y = Error(Variable)

Returns **1** if the variable is **not available** (error) or **0** if the variable is **available**. This function can be used to check variables for their existence.

Parameter

Variable

The variable to be tested.

Examples

- Error('Result 1.*Command name*') = 0: The result could be calculated.
- Error('Meas.EP(3).*Command name*') = 0: The variable for the measured value at equivalence point 3 exists.
- Error('Meas.EP(3).*Command name*') = 1: No variable for the measured value or no equivalence point 3 exists.

If a variable has an invalid value or the result of the variable could not be calculated, the function returns the value **0** as long as the variable is **available** in the system.

Example:

If the variable**'Result 1.*Command name*'** yields an invalid result, but is available, the variable will yield:

Error('Result 1.*Command name*') = 0

5.11.9.5.6 Exp – Exponential function

Syntax

y = Exp(number)

Calculates e ^ number. Other notation for $y = e^{(number)}$, where e is the Euler number (e = 2.71828…).

Parameter

Number (Exponent)

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.

Examples

- Exp(1.5) = 4.48169
- Exp('Temperature.EP{x}.*Command name*') = power of the exponent (Variable 'Temperature.EP{x}.*Command name*') to base e.

5.11.9.5.7 Floor – Rounding-down function

Syntax

y = Floor(number)

Returns the nearest integer that is less than or equal to the entered number.

Parameters

Number

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expec-

ted type, then the result of the operation will be returned as **invalid** and an error message will appear.

Examples

- Floor(2.9) = 2
- Floor(1.01) = 1
- Floor(3) = 3
- Floor(-1.1) = -2
- Floor(0) = 0

5.11.9.5.8 Length – Length of a character string

Syntax

- **y = Length("character string")**
  Outputs the number of characters of the **character string** as a number.

Parameters

Character string

Character string from which the number of characters is output.

Examples

- Length("Subsample") = 9
- Length("Sample") = 6

5.11.9.5.9 Log – Common logarithm

Syntax

y = Log(number)

Returns the logarithm of the entered number for base 10. Alternative notation for $y = \log_{10}$ (number).

Parameter

Number > 0

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.

Examples

- Log(10) = 1
- Log('Temperature.EP{x}.*Command name*') = common logarithm of the value of the variable 'Temperature.EP{x}.*Command name*'.

5.11.9.5.10 Ln – Natural logarithm

Syntax

y = Ln(number)

Returns the logarithm of the entered number for base e. Alternative notation for y = $\log_e$(number), where e is the Euler number (e = 2.71828…).

Parameter

Number > 0

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.

Examples

- Ln(3) = 1.09861
- Ln('Temperature.EP{x}.*Command name*') = natural logarithm of the value of the variable 'Temperature.EP{x}.*Command name*' to base e.

5.11.9.5.11 Max – Maximum

Syntax

y = Max(Number1;Number2)

Returns the larger element (Maximum) of the two values **Number1** and **Number2**.

A maximum of 2 values can be entered.

Parameter

Number

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.

Example

- Max(5;2) = 5

5.11.9.5.12 Min – Minimum

Syntax

y = Min(Number1;Number2)

Returns the smaller element (Minimum) of the two values **Number1** and **Number2**.

A maximum of 2 values can be entered.

Parameter

Number

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.

Example

- Min(5;2) = 2

5.11.9.5.13 NumberToText – Convert number to text

Syntax

y = NumberToText(number)

Returns the entered number as text.

Parameter

Number

The parameter can be indicated either directly as a number or as a variable of the **Number** type.

Example

- NumberToText(–55.3) = "–55.3"

5.11.9.5.14 Pow – Power

Syntax

y = Pow(number;exponent)

Calculates the power from the entered number and the entered exponent (number ^ exponent, e.g. 5^2).

Parameters

Number and **Exponent**

The parameters can be indicated either directly as a number or as a variable of the **Number** type. If the parameters do not correspond to the expected type, then the result of the operation will be returned as **invalid** and an error message will appear.

Examples

- Pow(5;2) = 25
- Pow(4;3) = 64

5.11.9.5.15 Rand – Generate random number

Syntax

- **y = Rand(p)**
  Returns a random number between 0 and 1 with **p** decimal places.
- **y = Rand(a;b;p)**
  Returns a random number between **a** and **b** with **p** decimal places.

Independently of the number of decimal places set in this function, a result is always output with the number of decimal places defined in the parameter **Decimal places**.

Parameter

Number, for which the following prerequisites must be fulfilled:

- **a** < **b**
- **p** ≤ 15

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.

Example

- Rand(1;5;2) = 3.54

5.11.9.5.16 RegEx – Regular expression

Syntax 1

- **y = RegEx(Text;"Regular expression")**
  Returns the fragment of the variable content that corresponds to the specifications of the regular expression.

Syntax 2

- **y = RegEx(Text;"Regular expression";Number)**
  Returns the fragment of the variable content that corresponds to the specifications of the regular expression. If several fragments correspond to the specifications, the third parameter **number** determines which number fragment should be used as a result.

The OMNIS Software uses the Regular Expression Package of the .Net framework. Further information on regular expressions and practical examples are available on the Internet, for example under the following link: *Wikipedia - Regular Expression*

Parameter

- **Variable**
  The parameter can be indicated either as a variable of the **Text** or of the **Number** type or directly as text. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **invalid** and an error message will appear.
  Variable: Entry with apostrophes '*Variable name*'
  Text: Entry with quotation marks "*Example text*"
- **Regular expression**
  The parameter has to correspond to a regular expressed and must be written in quotation marks. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **invalid** and an error message will appear.
- **Number**
  The numbering begins at 1. The parameter can be indicated either directly as a number or as a variable of the **Number** type. The parameter must be a whole number. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **invalid** and an error message will appear.

Examples for application

RegEx("12ABC34";"AB")	returns: AB
RegEx("12ABC34";"[0-9]")	returns: 1
RegEx("12ABC34";"[0-9]{1,}")	returns: 12
RegEx("12ABC34";"[A-Z]")	returns: A
RegEx('Variable1';"\d+")	returns: The first number with multiple digits
RegEx('Variable1';"\d";2)	returns: The second digit of a variable
RegEx("12.64ph";"\d{2}\.\d{2}")	returns: 12.64
RegEx("ABC";"BC|DE")	returns: BC
RegEx("ABC[DEF";"\[")	returns: [
RegEx("12ABC34";"[0-9]+")	returns: 12
RegEx("123ABC";"[^0-9]+")	returns: ABC
RegEx("ABC\DEF";"\\")	returns: \

Possible expressions

Regular expression	Description	Example

[abc]	OR function for individual characters	a or b or c
[a-z0-9]	Character, lowercase letter or digit	m or 5
(hallo)	Substring	String contains hallo
^hallo	Beginning of string	hallo is at the beginning of the string
hallo$	End of string	hallo is at the end of the string
.	Any character	a or 4 or - etc.
\.	Period	.
\d	Exactly one digit	1
\d+	All digits of a number sequence	1234567
\d{4}	Exactly 4 digits of a sequence	3143
\D	Not exactly one digit	A or ! etc.
\w	One digit or letter	a or 3
\W	Neither digit nor letter	returns: ! or .
.*	Any character string	abcd or 41 or -$=$ etc.

5.11.9.5.17 Replacing – Replace character string

Syntax

- **y = Replace("Character string1";"Character string2";"Character string3")**
  Replaces the **Character string2** in the **Character string1** with the **Character string3** and outputs the result as a new character string.

Parameters

Character string1

Original character string that contains the character string to be replaced.

Character string2

Character string that is to be replaced.

The character string1 must contain the character string2.

Character string3

Character string is replaced by the character string2.

Examples

- Replace ("SubsampleNew;"New";"Old") = SubSampleOld
- Replace ("SubsampleNew;"New";"") = SubSample

5.11.9.5.18 Round – Rounding

Syntax

- **y = Round(number; p)**
  Returns the rounded value of the entered number as a rounded number. The rounding is determined by the number of decimal places defined in the **p** parameter.

The number of decimal places set in this function only refers to rounding. When the result is displayed after the determination, the number defined in the **Decimal places** command parameter is taken into account.

Parameter

Number

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **invalid** and an error message will appear.

Rounding

OMNIS uses commercial rounding (according to DIN1333). This corresponds to the guidelines on rounding in the pharmacopeia of the United States (USP, United States Pharmacopeia) and in the European Pharmacopoeia (Ph. Eur., Pharmacopoea Europaea).

- If the last digit to be retained is followed by 1, 2, 3, 4, then it will be rounded down.
- If the last digit to be retained is followed by 5, 6, 7, 8, 9, then it will be rounded up.

Examples

- Round(–55.5259;0) = –56
- Round(–55.5259;2) = –55.53
- Round('Temperature.EP{x}.*Command name*';3) = Value of the variable 'Temperature.EP{x}.*Command name*' rounded to 3 decimal places.

See also

Functions – Directory (chapter 5.11.9.5, page 831)

5.11.9.5.19 Sign – Sign function

Syntax

y = Sign(number)

Returns **1** if the algebraic sign of the entered number is positive, returns **-1** if the sign is negative, or returns **0** if the entered number is 0. This function can be used to determine the algebraic sign of a number.

Parameters

Number

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **invalid** and an error message will appear.

Examples

- Sign(2.9) = 1
- Sign(-2.9) = -1
- Sign(0) = 0

5.11.9.5.20 Sqrt – Square root

Syntax

y = Sqrt(number)

Returns the square root of the entered number. Alternative notation for y = $\sqrt{}$ **number** or y = $^{2}\sqrt{}$ **number**.

Parameter

Number ≥ 0

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.

Examples

- Sqrt(33) = 5.745
- Sqrt('Temperature.EP{x}.*Command name*') = Square root of the value of the variable 'Temperature.EP{x}.*Command name*'.

5.11.9.5.21 SubText – Return part of a character string

Syntax

y = SubText(Text;Position;Character length)

Returns the part of text from **Text** that begins at the specified **Position** and has the specified **Character length**.

Parameter

- **Text**
  The parameter can be indicated either directly as text or as a variable of the **Text** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.
- **Position**
  The numbering of the position begins at 1. The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.
- **Length**
  The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type or if the length specified here is greater than the length of the subtext, then the result of the operation will be returned as **Invalid** and an error message will appear.

Examples

- SubText("Citric acid";8;4) = acid
- SubText("Citric acid";8;5) = invalid, only 4 characters exist from position 8 onwards

5.11.9.5.22 TextPosition – Return position of character string searched for

Syntax

y = TextPosition(Text;Sample text)

Returns the number of characters up to the first appearance of the **sample text** character string in the specified **text**.

Parameter

- **Text**
  The parameter can be indicated either directly or as a variable of the **Text** type.
- **Sample text**
  The parameter can be indicated either directly or as a variable of the **Text** type. If the **Sample text** is not included in the **Text**, then **0** is returned.

Examples

- TextPosition("AAA BBB CCC";"CCC") = 9, the word "CCC" occurs in the text from index number 9 onwards.
- TextPosition("Citric acid";"Acid") = 0, the word "Acid" (capitalized) does not occur in the text.

- TextPosition("Citric acid";"salt") = 0, the word "salt" does not occur in the text.
- TextPosition("3362.14";"6") = 3, because the number "6" is in third position.

5.11.9.5.23 TextToNumber – Convert text to number

Syntax

y = TextToNumber(Text)

Returns the entered text as a number. This makes it possible, for example, to use character strings of external instruments for the calculation.

Parameter

Text

The parameter may only contain numerical characters or variables of the **Text** type, as otherwise a type conversion is not possible. The result of this conversion or calculation, respectively, would be in this case **Invalid**. In addition, text must be marked by quotation marks.

Example

- TextToNumber("–55") = –55

5.11.9.5.24 Time – Time

Syntax

- **y = Time()**
  Returns the current date and the current time as text in the format 'YYYY-MM-DD hh:mm:ss'.
- **y = Time(Year;Month;Day)**
  Returns the date as text in the format 'YYYY-MM-DD'.
- **y = Time(Year;Month;Day;Hour;Minute;Second)**
  Returns the date and the time as text in the format 'YYYY-MM-DD hh:mm:ss'.

Parameter

Number > 0

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **Invalid** and an error message will appear.

Examples

- Time(2016;03;25) = 2016-03-25
- Time(2015;05;08;16;43;26) = 2015-05-08 16:43:26

5.11.9.5.25 TimeToNumber – Convert date/time to number

Syntax

- **y = TimeToNumber(Time())**
  Returns the current date and the current time as a number.
- **y = TimeToNumber("Year-Month-Day")**
  Returns the entered date as a number.
- **y = TimeToNumber(Time("Year-Month-Day"))**
  Returns the entered date as a number.
- **y = TimeToNumber(Time(Year;Month;Day))**
  Returns the entered date as a number.
- **y = TimeToNumber(Time("Year-Month-Day Hour:Minute:Second"))**
  Returns the entered date and the entered time as a number.
- **y = TimeToNumber("Year-Month-Day Hour:Minute:Second")**
  Returns the entered date and the entered time as a number.
- **y = TimeToNumber(Time(Year;Month;Day;Hour;Minute;Second))**
  Returns the entered date and the entered time as a number.
  The number is calculated as the number of days from 01.01.1900 to the current or entered date/time.

The local time is always used for the calculation.

Parameters

Date/Time

Either the date or date and time or variables of the **Date/time** type can be specified directly as parameters.

Examples

- TimeToNumber(Time()) = 45221
- TimeToNumber(Time(2023;08;10)) = 45145.96
- TimeToNumber(Time(2023;08;10;16;43;26)) = 45146.66
- TimeToNumber('CreationTimestamp.CurrentSubsampleData') = 45199.65
- TimeToNumber("2023-08-10") = 45145.96
- TimeToNumber(Time("2023-08-10")) = 45145.96
- TimeToNumber(Time("2023-08-10 16:43:26")) = 45146.66
- TimeToNumber("2023-08-10 16:43:26") = 45146.66

5.11.9.5.26 TimeToText – Convert date/time to text

Syntax

- **y = TimeToText(Time())**
  Returns the current date and the current time as text.
- **y = TimeToText(Time(Year;Month;Day))**
  Returns the entered date as text.
- **y = TimeToText(Time(Year;Month;Day;Hour;Minute;Second))**
  Returns the entered date and the entered time as text.
- **Concat(TimeToText(Time());" Text1")**
  Combines the current date and current time as text with Text1 to form a new complete text.

The local time is always used for the calculation.

Parameters

Date/Time

Either the date or date and time or variables of the **Date/time** type can be specified directly as parameters.

Example

- TimeToText(Time()) = "2023-08-10 10:05:51"
- TimeToText(Time(2023;08;10)) = "2023-08-10"
- TimeToText(Time(2023;08;10;16;43;26)) = "2023-08-10 16:43:26"
- Concat(TimeToText(Time());" Text") = "2022-05-23 10:23:51 Text"
- TimeToText('CreationTimestamp.CurrentSubsampleData') = "2015-05-08 16:23:26"

5.11.9.5.27 Trim – Remove blank spaces / character string

Syntax

- **y = Trim(Text)**
  Returns the **text** without spaces before and after.
- **y = Trim(Text;Sample text)**
  Returns the **text** without **sample text**.

Parameter

- **Text**
  The parameter can be indicated either directly or as a variable of the **Text** type.
- **Sample text**
  The parameter can be indicated either directly or as a variable of the **Text** type.

Examples

- Trim("Citric acid") = Citric acid

- Trim("Citric acid";"acid") = Citric
- Trim("Citric acid";"salt") = Citric acid

5.11.9.5.28 Truncate – Truncate to integer

Syntax

y = Truncate(number)

Returns the entered number truncated to an integer by eliminating the decimal places.

Parameters

Number

The parameter can be indicated either directly as a number or as a variable of the **Number** type. If the parameter does not correspond to the expected type, then the result of the operation will be returned as **invalid** and an error message will appear.

Examples

- Truncate(2.9) = 2
- Truncate(-2.9) = -2
- Truncate(0.23) = 0

5.11.10 Text editor – Brief description

The text editor is used for the entry and formatting of message texts and notifications. Graphics can also be added.

If text is entered, the amount must not exceed 10 A4 pages.

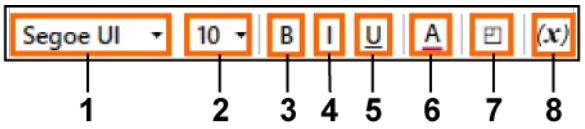
Commands

The text editor is available in the commands **WAIT**, **REQUEST** and **NOTIFY** for the entry of individual text messages.

The text editor can be opened by clicking on **[Edit message]** or **[Edit notification]** in the **Parameters** subsection of the **Properties** window in the respective command.

Editor – Formatting elements

The following formatting elements are used to format elements within the message or notification:



1	**Font** Selection of the font for the text through the selection menu of the installed Windows system fonts.
2	**Font size** Selection of the text size for the text through the selection menu.
3	**Bold** The text is displayed in bold.
4	**Italic** The text is displayed in italics.
5	**Underline** The text is displayed underlined.
6	**Text color** The text is displayed in color. A dialog window opens in which a text color can be selected.
7	**Insert graphic (recommended file formats: JPG, PNG)** A graphic can be inserted. The graphics file can be selected from a directory in the Explorer window.
8	**Inserting a variable (only available in the NOTIFY command)** A variable can be entered as a placeholder in a notification. When the notification is sent, the variable is replaced with real data.

Basic editing options

The basic editing options of the Windows operating system (Windows OS) used are available in the editor. For example, a highlighted text can deleted by clicking on **[(Delete)]**.

The display size of the image can be modified. To do this, position the cursor at one of the editing points at the edge of the image and keep the left mouse button pressed while moving the cursor.

See also

NOTIFY – Parameters (chapter 5.11.8.72, page 787)

REQUEST – Parameters (chapter 5.11.8.77, page 794)

WAIT – Parameters (chapter 5.11.8.84, page 807)

5.12 Equipment – Actions

You can trigger the following actions in the subsections of the **Equipment** work area:

-
  Instruments used for analysis are reserved in **Equipment** ▶ **Instruments**. The instruments can also be released again so that other users will be able to access them.
-
  Work systems are assembled from functional units in **Equipment** ▶ **Work systems**. The work systems can be assigned the methods which are used for the analyses.
-
  The automatically detected digital sensors and the manually created analog sensors are managed in **Equipment** ▶ **Sensors**.
-
  The automatically recognized solutions and conductivity standards are managed in **Equipment** ▶ **Solutions**.
-
  The automatically recognized sample racks and the imported sample racks are managed in **Equipment** ▶ **Sample racks**.
-
  Calibration buffers for the calibration of pH electrodes are defined in **Equipment** ▶ **Custom calibration buffers**.
-
  External standards for the reference standardization of spectrometers are imported and managed in **Equipment** ▶ **Standards**.

See also

Calibration buffers – Definition (chapter 5.12.9, page 1034)

Instruments – Definition (chapter 5.12.2, page 853)

Sample rack – Definition (chapter 5.12.8, page 1023)

Sensor – Definition (chapter 5.12.6, page 998)

Solution – Definition (chapter 5.12.7, page 1012)

Standards – Subsection (chapter 5.12.11, page 1050)

Work system – Definition (chapter 5.12.4, page 987)

5.12.1 Equipment – Inventory

This topic describes the **Inventory** window in the **Instruments**, **Sensors** and **Solutions** subsections of the **Equipment** work area, and on the **Work system** tab.

Clicking on opens the **Inventory** window. In this window, instruments, functional units, analog sensors and conductivity standards are displayed for solutions and can be selected. Drag and drop to reserve the displayed instruments, add sensors to the sensor list, solutions to the solution list, and functional units to the work system.

The **Inventory** window of the **Instruments** subsection lists **Network instruments** and **Other instruments**.

Select the **Other instruments** area to display instruments that are connected via a serial interface.

When the **Network instruments** area is selected, all instruments connected in the network are displayed. In this area, instruments that are assigned to other subnets and cannot be found automatically can additionally be added manually and removed again as required.

Information on the functions of the available icons in the **Inventory**: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)* window:

After a work system has been selected or assembled, all functions units available on the reserved instruments are displayed on the **Work system** tab in the **Work systems** subsection. These functional units can be added to the work system via drag and drop.

Search function

There is a search function in **Equipment** ▶ **Instruments** ▶ **Inventory**. If the name, the type or the IP address of the required **instrument** is known, then one of these search criterion can be entered in the search field. The resulting list will then include only those instruments that fulfil the entered search criteria.

See also

Creating a work system (chapter 5.12.4.4, page 989)

Functional unit – Directory (chapter 5.12.3.1, page 894)

Instruments – Directory (chapter 5.12.2.2, page 854)

Ion-selective electrode – Calibrating (chapter 5.12.6.5, page 1010)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Reserving and releasing instruments (chapter 5.12.2.4, page 861)

Sensor – Definition (chapter 5.12.6, page 998)

Sensor – Properties (chapter 5.12.6.2, page 1001)

Solution – Definition (chapter 5.12.7, page 1012)

pH electrode – Calibrating (chapter 5.12.6.4, page 1008)

5.12.2 Instruments – Definition

Instruments are used for performing analyses. They are connected either via a network connection (e.g. OMNIS instruments) or directly to a computer (e.g. USB device) that runs the OMNIS Software. An instrument is comprised of one or more functional units that can be combined to form a work system independently of one another. An instrument remains available for all users in the network until it is reserved by a user.

See also

Backing up instrument data (chapter 5.12.2.7, page 867)

Equipment – Inventory (chapter 5.12.1, page 852)

Instruments – Directory (chapter 5.12.2.2, page 854)

Instruments – Manual control (chapter 5.12.2.6, page 867)

Instruments – Properties (chapter 5.12.2.5, page 865)

Instruments – Status (chapter 5.12.2.3, page 859)

Reserving and releasing instruments (chapter 5.12.2.4, page 861)

5.12.2.1 Instruments – Subsection

Instruments can be reserved under **Equipment** ▶ **Instruments**. Furthermore, the following functions are available:

-

  Use **Save** to save all changes.
-

  Remove instruments is used to remove the instrument, thus releasing it once again. Work systems which were created with this instrument are retained.

In addition, the following windows can be opened:

-

  The selection of all available instruments is displayed in the **Inventory** window.
-

  The selected functional unit cannot be operated manually in the **Manual control** window.

-

  The properties of the selected element are displayed in the **Properties** window.

See also

Instruments – Definition (chapter 5.12.2, page 853)

Instruments – Directory (chapter 5.12.2.2, page 854)

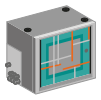
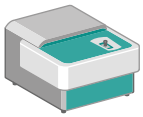
Instruments – Status (chapter 5.12.2.3, page 859)

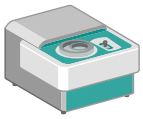
Reserving and releasing instruments (chapter 5.12.2.4, page 861)

5.12.2.2 Instruments – Directory

- *OMNIS instruments*
- *Metrohm USB instruments*
- *Other instruments*

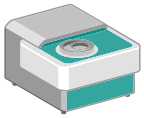
OMNIS instruments

	**2060 The NIR** The spectrometer can be used for near-infrared spectroscopic analysis in a process environment.
	OMNIS Coulometer The coulometer can be used for coulometric Karl Fischer titrations, bromine index determinations, and measurements of both potential and temperature.
	OMNIS Coulometer Module The coulometer module can be used for automated sample analysis. It can be used only in combination with an **OMNIS Coulometer** or an **OMNIS Titrator** and extends the **titration system** to include an additional measuring input.
	OMNIS Dosing Module The dosing module can be used for dosing solutions. It can be used only in combination with an **OMNIS Coulometer**, **OMNIS Titrator** or an **OMNIS Sample Robot** and extends the **titration system** to include an additional dosing unit.
	**OMNIS NIR Analyzer Liquid** The spectrometer with liquid sample presentation can be used for near-infrared spectroscopic analysis with the transmission measuring principle.



OMNIS NIR Analyzer Liquid/Solid

The spectrometer with liquid sample presentation and solid sample presentation can be used for near-infrared spectroscopic analyses with the measuring principles of transmission, reflection and transflection.

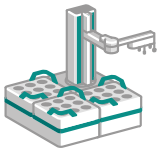


OMNIS NIR Analyzer Solid

The spectrometer with solid sample presentation can be used for near-infrared spectroscopic analyses with the measurement principles of reflection and transflection.

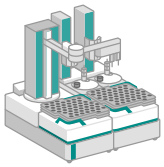
OMNIS Sample Robot

The sample robot can be used for automated sample processing for titrations and spectroscopic measurements.



OMNIS Sample Robot NIR

The sample robot can be used for automated sample processing in spectroscopic analyses.



OMNIS Sample Robot Oven

The sample robot with oven module can be used for automated thermal water extraction in Karl Fischer titrations.

OMNIS Solvent Module

The solvent module can be used in combination with an **OMNIS Coulometer** or **OMNIS Titrator** in stand-alone operation or in an automated analysis system for liquid handling tasks.

OMNIS Titration Module

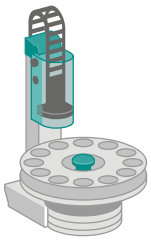
The titration module can be used for automated sample analysis. It can be used only in combination with an **OMNIS Coulometer** or **OMNIS Titrator** and extends the **titration system** to include an additional dosing unit and up to 2 measuring inputs.

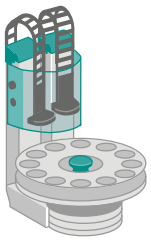
OMNIS Titrator

The titrator can be used for equivalence point titrations, endpoint titrations, and volumetric Karl Fischer titrations, as well as for concentration, conductivity, pH value, potential, and temperature measurements.

Metrohm USB instruments

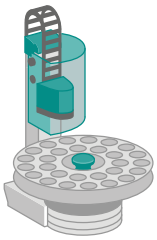
Metrohm USB instruments must be connected to the same computer as the one on which the OMNIS Software is installed.

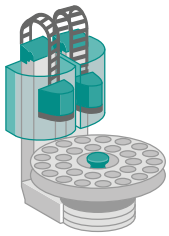




814 USB Sample Processor

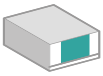
The sample changer can be used for automated sample processing of titrations and measurements.





815 Robotic USB Sample Processor XL

The sample changer can be used for automated sample processing of titrations and measurements.



846 Dosing Interface

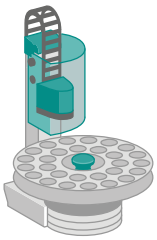
The dosing interface is used as the interface for multiple functional units of the MSB dosing device, MSB stirrer or Remote Box MSB types and can be used for dosing auxiliary solutions.

851 Titrando

The titrator can be used for coulometric Karl Fischer titrations and potential and temperature measurements.

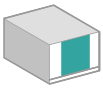
852 Titrando

The titrator can be used for volumetric and coulometric Karl Fischer titrations as well as for potential and temperature measurements.



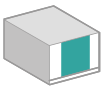
855 Robotic Titrosampler

The sample changer with integrated titrator can be used for automated sample processing as well as for equivalence point titrations, endpoint titrations and for the measurement of concentration, pH value, potential and temperature.



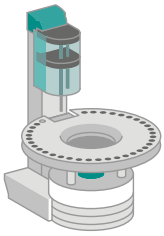
856 Conductivity Module

The conductivity measuring module can be used for conductivity measurements and for calibrating conductivity measuring cells.



867 pH Module

The pH module can be used for measuring the pH value, concentration, potential and temperature as well as for calibrating pH electrodes and ion-selective electrodes.



874 Oven Sample Processor

The sample changer can be used for automated thermal water extraction in Karl Fischer titrations.

888 Titrando

The titrator can be used for volumetric Karl Fischer titrations, potentiometric titrations as well as pH value, potential and temperature measurements.

890 Titrando

The titrator can be used for volumetric Karl Fischer titrations as well as for potential measurements.

901 Titrando

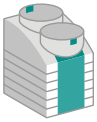
The titrator can be used for volumetric Karl Fischer titrations, endpoint titrations as well as pH value, potential and temperature measurements.

902 Titrando

The titrator can be used for endpoint titrations, pH value, potential and temperature measurements as well as enzymatic and STAT titrations.

904 Titrando

The titrator can be used for potentiometric and voltametric titrations, endpoint titrations as well as concentration, pH value, potential and temperature measurements.

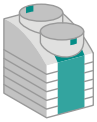


905 Titrando

The titrator can be used for potentiometric and voltametric titrations, endpoint titrations as well as concentration, pH value, potential and temperature measurements.

906 Titrando

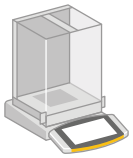
The titrator can be used for potentiometric and voltametric titrations, endpoint titrations, volumetric Karl Fischer titrations as well as concentration, pH value, potential and temperature measurements.



907 Titrando

The titrator can be used for potentiometric and voltametric titrations, endpoint titrations, volumetric Karl Fischer titrations as well as concentration, pH value, potential and temperature measurements.

Other instruments

	Balance The balance can be used for weighing in samples and for entering further sample data. The balance is connected to the OMNIS system via the RS-232 interface or the Ethernet network.
	**Cubis II Balance** The balance can be used for weighing in samples and for entering further sample data. The complete sequence of steps for weighing can be executed directly on the balance, if an instrument of the **Cubis II Balance** type from the balance series from Sartorius is used.
	Serial Device An instrument can be connected to the serial interface via RS-232 interface.

See also

Backing up instrument data (chapter 5.12.2.7, page 867)

Equipment – Inventory (chapter 5.12.1, page 852)

Functional unit – Directory (chapter 5.12.3.1, page 894)

Instruments – Manual control (chapter 5.12.2.6, page 867)

Instruments – Properties (chapter 5.12.2.5, page 865)

Instruments – Status (chapter 5.12.2.3, page 859)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Reserving and releasing instruments (chapter 5.12.2.4, page 861)

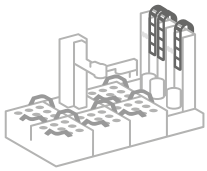
5.12.2.3 Instruments – Status

The icons of the instruments are displayed differently, depending on their status. In addition, all instruments that can be actively actuated are equipped with a status lamp. The color of the status lamp varies, depending on the status of the instrument.

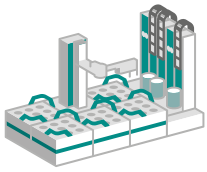
The status of the instruments in the OMNIS Software is represented as follows:

The icons and the colors of the status lamp are described in the following sections using the sample robot as an example.

Display in the Inventory



The instrument is reserved by another OMNIS system and is thus not available.

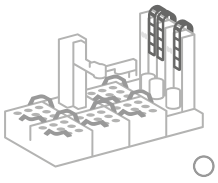


The instrument is available.

Display in overview of the instrument and work system

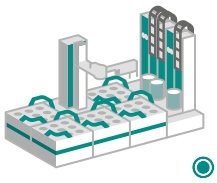
Network instruments can only be assigned to one OMNIS system. They are then reserved and no longer available for other systems.

Other instruments such as balances or barcode readers can be assigned to several OMNIS systems at the same time.

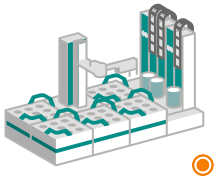


The instrument is not available. It is reserved by another OMNIS system or not connected to the power grid or not connected to the network.

On an instrument on which logging in is necessary, the grayed out status shows that it is connected to another OMNIS system and logging in is therefore not possible.



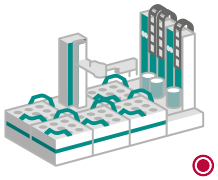
The instrument is connected to the OMNIS system and ready for operation.



The instrument is assigned to the OMNIS system, but it must be initialized.

On an instrument on which logging in is necessary, the orange status shows that it is not connected to any OMNIS system and that logging in is therefore possible.

For instruments of the **2060 The NIR** type and instruments in the **OMNIS NIR Analyzer** product family, orange status can **also** mean that the instrument has been restarted but that the start process is not yet completed.



The instrument is currently in the error state.

See also

Instruments – Directory (chapter 5.12.2.2, page 854)

Reserving and releasing instruments (chapter 5.12.2.4, page 861)

5.12.2.4 Reserving and releasing instruments

Under **Equipment** ▶ **Instruments**, instruments can be found automatically or added manually to reserve them as needed. The automatic search is carried out in all network segments that the computer has access to. This is also the case if the computer has multiple NICs or a wireless connection. If instruments cannot be found automatically because they are located in another subnet, then these instruments can be added manually. The instruments can be reserved; released and manually added instruments can be removed. After the reservation, the instruments are displayed together with their functional units and the additionally connected equipment (stirrers, solutions, sensors, sample racks, etc. in the subsection).

- *Searching for instruments automatically*
- *Adding instruments manually*
- *Reserving instruments*
- *Releasing instruments*
- *Removing manually added instruments*

- The user must have the necessary rights for searching for, adding, reserving and releasing instruments. Additional information on user rights: *Metrohm Knowledge Base*
- The necessary software licenses and function licenses must be enabled. Additional information: *Metrohm Knowledge Base*

Searching for instruments automatically

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The instrument in question is connected to the local network (OMNIS instruments).
  or

- The instrument in question is connected directly to the computer on which the OMNIS Software is installed (Metrohm USB instruments).

1 Opening inventory

- Open the **Equipment** ▶ **Instruments** subsection.
- Click on to open the **Inventory** window.

2 Searching for available instruments

- Select **Network instruments** or **Other instruments** in the selection list.

  If necessary, click on if new instruments have been connected.
- If desired, enter the desired search criterion (name, type, IP address) in the search field to filter the instruments.

The instruments in the network are displayed.

NOTICE: The instruments found are listed in the **Network instruments** area under **Automatically found instruments**.

Instruments with grayed-out icons cannot be reserved.

Adding instruments manually

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The instrument is assigned to a different subnet.
  or
- The instrument is connected directly to the computer on which the OMNIS Software is installed (only OMNIS devices, incl. the balance Cubis II Balance).
- The instrument has a static IP address: *(see "Assigning IP addresses", chapter 4.8, page 138)*

1 Opening inventory

- Open the **Equipment** ▶ **Instruments** subsection.
- Click on to open the **Inventory** window.

2 Adding instrument manually

- Select the **Network instruments** area in the selection list.
- Add an instrument from another subnet by clicking on +.

The instrument appears in the **Inventory** window under **Manually added instruments** and the **Properties** window opens.

3 Entering IP address

- Enter the IP address of the instrument in the **IP address** field. The entry must have the following format: E.g. 192.0.2.235.

The **[Check connection]** button appears at the bottom of the **Properties** window.

4 Checking connection

- Click on **[Check connection]**.
- If the connection to the instrument was able to be established, then the instrument will appear with the associated icon and instrument data such as product name and serial number will be updated. The instrument can be reserved.
- If the connection to the instrument was not able to be established, then an error message will appear.
  Check the IP address or its format and re-enter if necessary. Run the connection test again.

Reserving instruments

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The instrument is available in the **Inventory** window: *Searching for instruments automatically* or *Adding instruments manually*

1 Reserving instruments

- Drag and drop the instrument into the adjacent work surface.

The instrument and the associated functional units are automatically reserved for this OMNIS system and locked for all other OMNIS systems.

A green status lamp next to the instrument indicates that the instrument can be used.

The instruments are reserved by the **Metrohm Miami LabLogic** service. This service is installed together with the OMNIS Software and starts automatically when starting Windows. This means that the instruments remain reserved, even if the OMNIS Software is exited.

The instruments are released once they are manually released in the OMNIS Software or if the **Metrohm Miami LabLogic** service is stopped or if the computer is switched off.

If the **Metrohm Miami LabLogic** service is stopped unexpectedly, e.g. due to a power failure, then instruments can sometimes no longer be found in the network. In this case, this service needs to be restarted under "Services" in the Windows Task Manager. A search for instruments on the network can then be started again and they can be reserved: *Start services*

Releasing instruments

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The instrument is reserved: *Reserving instruments*

1 Opening instrument management

- Open the **Equipment** ▶ **Instruments** subsection.

2 Releasing instruments

- Select the reserved instrument.
- Release the selected instrument by clicking on ✕ or by pressing the **[DELETE]** key.

The instrument and the associated functional units are released and available for all other OMNIS systems.

Removing instruments added manually

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

- The instrument is available under **Manually added instruments**: *Adding instruments manually*

1 Opening inventory

- Open the **Equipment** ▶ **Instruments** subsection.
- Click on to open the **Inventory** window.

2 Removing a manually added instrument

- Select the instrument added in the **Inventory** window.
- Remove the selected instrument by clicking on or by pressing the **[DELETE]** key.

The instrument is no longer available in the **Inventory** window.

See also

Activating the function license (chapter 4.2.3, page 35)

Equipment – Inventory (chapter 5.12.1, page 852)

Instruments – Manual control (chapter 5.12.2.6, page 867)

User rights – Directory (chapter 4.5.7.4, page 89)

5.12.2.5 Instruments – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 3 subsections **General**, **Specific data** and **Licenses and firmware**:

General

Product information	
Product name	Name of the instrument or the functional unit (max. 150 characters). If the instrument or the functional unit contains a memory chip, the name is stored there and is retained. If the instrument or functional unit does not contain a memory chip, the name is stored on the local computer. If the instrument is connected to another computer, the default name is displayed.
Product type	Display the English designation of the instrument properties.

Production data	
Article number	Number that identifies the product unambiguously. For balances, the article number must be entered by the user if it is to be recognized in the software in other areas, e.g. in the subsample history or in the Audit Trail.
Serial number	Serial number of the product. For balances or serial instruments, the serial number must be entered by the user if it is to be recognized in the software in other areas, e.g. in the subsample history or in the Audit Trail.

If an OMNIS instrument is selected, the following parameter group also appears:

Instrument data	
Back up instrument data	Back up the current state of the instrument data. In case of an error, the data can be restored by the regional Metrohm service representative.

Specific data

Specific settings can also be made in this subsection if a functional unit has been selected.

Further information on the specific data of a functional unit can be found in the respective topic about that functional unit.

Licenses and firmware

License-dependent instrument functions can be activated in this subsection if an OMNIS instrument has been selected. For this, the licensing wizard carries out the sequence step by step. The firmware can also be updated in this subsection and the log files can be collected in the event of a malfunction.

The information in the **Licenses and firmware** subsection is only valid for OMNIS instruments. No licensing is needed to use the instrument functions of Metrohm USB devices.

Modified data of the instrument or of the functional unit cannot be saved for as long as it is being used by a method in the process sequence.

See also

Backing up instrument data (chapter 5.12.2.7, page 867)

Collecting instrument log files (chapter 7.4, page 1241)

5.12.2.6 Instruments – Manual control

The **Manual control** can be used to actuate a reserved instrument directly, i.e. without pre-defined operating procedure. The prerequisites for this are:

- The instrument is switched on.
- The instrument is recognized by the OMNIS Software.
- The instrument is reserved under **Equipment** ▶ **Instruments**.
- The instrument is not occupied by a process sequence.

Opening the manual control

Click this icon to open the **Manual control** of the selected instrument. Alternatively, double-click the required instrument.

Functions with icons

Click on this icon to initialize or restart the instrument.

Note: Clicking on this icon restarts only instruments of the **2060 The NIR** type and instruments of the **OMNIS NIR Analyzer** product family.

See also

2060 The NIR – Manual control (chapter 5.12.2.10.1, page 873)

Functional unit – Manual control (chapter 5.12.3.5, page 906)

OMNIS NIR Analyzer Liquid – Manual control (chapter 5.12.2.10.2, page 874)

OMNIS NIR Analyzer Liquid/Solid – Manual control (chapter 5.12.2.10.4, page 877)

OMNIS NIR Analyzer Solid – Manual control (chapter 5.12.2.10.3, page 876)

Sample robot – Manual control (chapter 5.12.2.8, page 868)

5.12.2.7 Backing up instrument data

Make sure that the connection to the instrument is not interrupted during the backup. The instrument must not be switched off or changed.

Back up the instrument data before every update of the OMNIS Software and after every firmware update.

1 Opening Instrument management

- In the **Equipment** work area, open the **Instruments** subsection.

2 Selecting the instrument

- Select the affected instrument by clicking on the title bar with the instrument name.

The depiction of the selected instrument with its functional units is shown with a green frame.

3 Opening the area

- Click on to open the **Properties** window.
- In the **Properties** window, select the **General** subsection.

4 Backing up instrument data

- Click on **[Back up instrument data]**.

The backup file is created in the **...ProgramData\Metrohm \OMNIS\DeviceBackup** directory.

The directory with the backup files is hidden by default in Windows.
The instrument data must be restored by a regional Metrohm service representative.

Repeat steps 1 to 4 for all available instruments.

See also

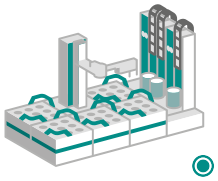
Instruments – Definition (chapter 5.12.2, page 853)

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.2.8 Sample robot – Manual control

If an instrument of the **OMNIS Sample Robot**, **OMNIS Sample Robot NIR** or **OMNIS Sample Robot Oven** type is selected in the **Instruments** subsection, then the information and **Initialization** function available for the instrument are displayed in the **Manual control** window.

Status display



The depiction of the instrument and the color of the status lamp represent the current status of the sample robot: *Instrument status*.

Initializing

	Click this icon to initialize the sample robot with all associated functional units. The status lamp of the sample robot lights up **orange** during the initialization. Once all of the associated functional units have been initialized, the status lamp will lights up **green**.

The entire gripper arm of the sample robot must be within the instrument limits for the instrument to be initialized. The instrument limits are defined by the rack base.

If the gripper arm is outside this area, then it needs to be moved back manually into this area.

See also

Gas Flow Unit – Manual control (chapter 5.12.3.19.2, page 955)

Main module – Manual control (chapter 5.12.3.15, page 941)

OMNIS NIR Analyzer Liquid – Manual control (chapter 5.12.2.10.2, page 874)

OMNIS NIR Analyzer Liquid/Solid – Manual control (chapter 5.12.2.10.4, page 877)

OMNIS NIR Analyzer Solid – Manual control (chapter 5.12.2.10.3, page 876)

Oven Module – Manual control (chapter 5.12.3.18.1, page 949)

Oven Unit – Manual control (chapter 5.12.3.19.1, page 954)

Pick&Place Module – Manual control (chapter 5.12.3.20.1, page 956)

Pump module – Manual control (chapter 5.12.3.27, page 966)

5.12.2.8.1 874 Oven Sample Processor – Faults

If an error occurs on an instrument of the **874 Oven Sample Processor** type, then the error message **030159** will be displayed, which contains a corresponding error code. If the error cannot be rectified by restarting the instrument, then contact must be made with the regional Metrohm representative. The following errors could occur:

Error code	Cause
013-001-1-255	Communication problems exist between the oven unit and the sample changer.

Error code	Cause
013-002-1-255	The data of the oven unit cannot be processed by the sample changer.
013-003-1-255	The diagnostics function takes too long.
013-004-1-255	The value defined for the gas flow is not achieved.
013-005-1-255	The temperature or the gas flow cannot be measured because the A/D converter is defective.
013-006-1-255	The sample changer has been switched off in the interests of safety because the maximum temperature was exceeded.
013-007-1-255	The temperature sensor is defective or not connected.
013-008-1-255	The adjustment data is faulty or not available.

See also

Oven / Gas Flow Unit – Properties (chapter 5.12.3.19, page 953)

5.12.2.9 Serial instrument – Properties

After selecting the **Serial Device** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for the **RS-232 configuration** in the **Specific data** subsection:

RS-232 configuration	
COM port	Display of the serial interface on the computer to which the data is transferred.
Baud rate	Transfer rate. The baud rate selected here must correspond with the baud rate set on the instrument.
Data bit	Number of data bits.
Parity	Type of parity testing.
Stop bit	Number of stop bits.
Handshake	Type of the data transfer protocol.

RS-232 configuration	
Maximum waiting time	Maximum waiting time for receiving characters. If this time is exceeded, receiving will be canceled.
Terminator for send	Terminator for sending in hexadecimal code (**\0D** = CR (carriage return), **\0A** = LF (line feed).
Terminator for receive	Terminator for receiving in hexadecimal code (**\0D** = CR (carriage return), **\0A** = LF (line feed).
Code page	Code page used for the data transfer.

Additional parameters	
Sending characters separately	If this option is activated, then each character is sent individually and the waiting time has to elapse before the next character is sent.
Waiting time	Waiting time until the next character is sent.

Button	
[Check connection]	Checks the connection between the serial interface and the serial instrument.

See also

Configuring the balance (chapter 5.12.2.12.1, page 884)

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.2.10 Spectrometer – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window.

General

The product information and production data of the spectrometer are displayed in the **General** subsection. In addition, in this area there is the possibility of saving the current status of the instrument data: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*.

Specific data

The following functions and information are available in the **Specific data** subsection, depending on the instrument selected:

Channel 1–5 (only for 2060 The NIR)	
Measuring mode	Select measuring mode or disable the channel. ▪ **Off**: This channel is not used. ▪ **Transmission**: The light that goes through the sample is measured. ▪ **Reflection**: The light that is reflected by the sample is measured. ▪ **Transflection**: The light that goes through the sample and is reflected is measured.
Probe article number	Enter the number that identifies the probe unambiguously.
Probe serial number	Enter the serial number of the probe.
Fiber type	Select the fiber type that is used for the measurement. Depending on the selection of the measuring mode, different fiber types are available: ▪ Measurement through a single fiber: – **Single fiber 600 µm** – **Single fiber other** ▪ Measurement through a fiber bundle: – **Microbundle reflectance 37/37** – **Microbundle reflectance 37/7** – **Microbundle transmission 37+37** – **Microbundle NC 90/15**
Fiber article number	Enter the number that identifies the fiber optic unambiguously.
Fiber length	Enter the length of the fiber optic cable used.
Saved	Display the time of the last change.

Any change in the data of a channel necessitates a new calibration. Without recalibration, the channel cannot be used for measurements.

Lamp module	
Article number	Show the number that unambiguously identifies the product.
Serial number	Show the serial number of the product.
Hours	Show the operating hours of the lamp module.

Licenses and firmware

In this subsection, license-dependent instrument functions can be enabled, firmware updates can be carried out and the log files can be collected in the event of a malfunction: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*.

See also

Command – Directory (chapter 5.11.8.87, page 810)

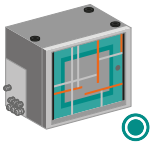
Instruments – Properties (chapter 5.12.2.5, page 865)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

5.12.2.10.1 2060 The NIR – Manual control

The following functions and information are displayed in the **Manual control** window for a reserved instrument of the **2060 The NIR** type:

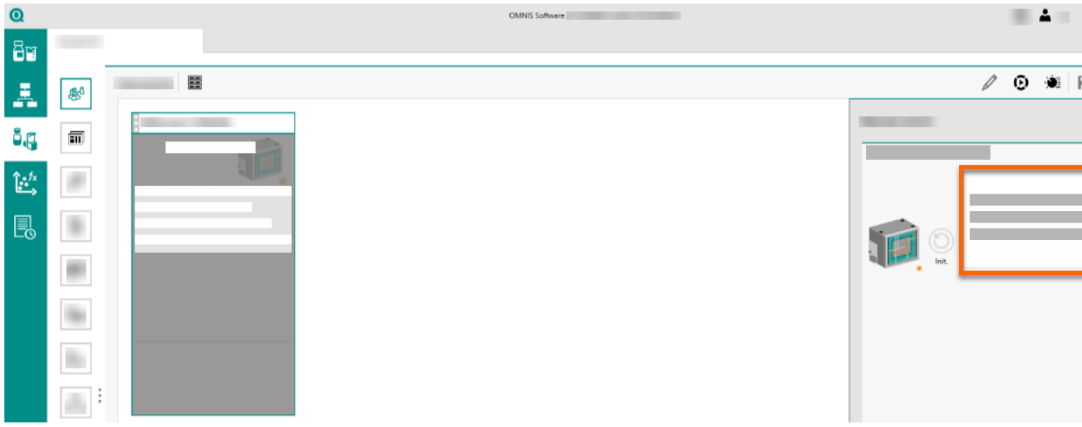
Status display



The depiction of the instrument and the color of the status lamp represent the status of the spectrometer: *Instrument status*.

Start process of the spectrometer

As soon as the spectrometer is switched on and the start process begins, the status window of the manual operation displays the status and the duration of the start process so far. The spectrometer cannot be operated during the start process. This may take up to 20 minutes.



Restart (Init.)

	Click this icon to restart the spectrometer. The icon, the depiction of the instrument and the status lamp are grayed out briefly during the restart. Afterwards, the status lamp lights up **orange** and the depiction of the instrument appears once again in color. The status window with the information on the start process is displayed. Once the restart is complete, the icon will reappear in color and the status lamp will light up **green**. The status window is hidden.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

Instruments – Manual control (chapter 5.12.2.6, page 867)

Instruments – Status (chapter 5.12.2.3, page 859)

5.12.2.10.2 OMNIS NIR Analyzer Liquid – Manual control

The following functions, parameters, and information are displayed in the **Manual control** window for a reserved instrument of the **OMNIS NIR Analyzer Liquid** type:

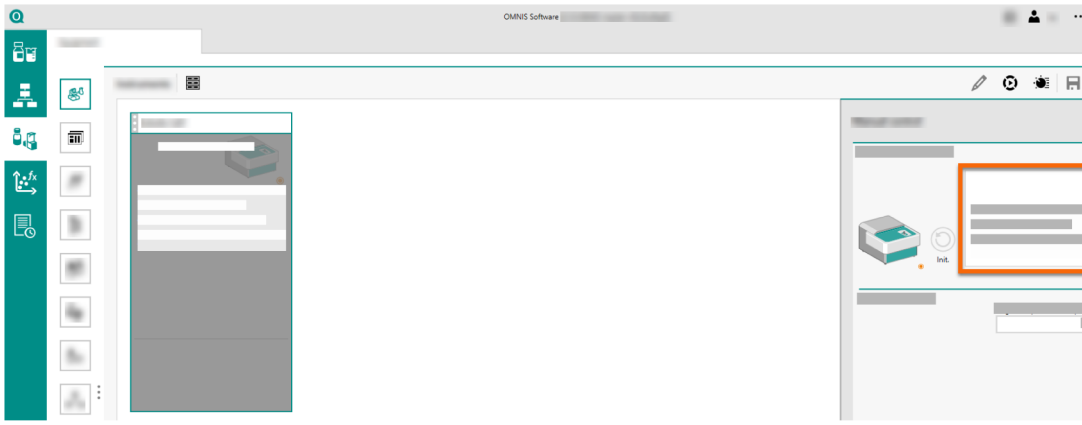
Status display and status window

The depiction of the instrument and the color of the status lamp represent the status of the spectrometer: *Instrument status*. Additionally, the status and the duration of the start process is displayed in the status window, along with the following information:

Target temperature sample holder or **Target temperature sample vessel**	Depending on the setting, the temperature that is controlled on either the sample holder or the sample vessel is displayed.
Temperature sample holder or **Temperature sample vessel**	Depending on the setting, the temperature currently reached on either the sample holder or the sample vessel is displayed.

Start process of the spectrometer

As soon as the spectrometer is switched on and the start process begins, the status window of the manual operation displays the status and the duration of the start process so far. The spectrometer cannot be operated during the start process. This may take up to 20 minutes.



Restart (Init.)

	Click this icon to restart the spectrometer. The icon, the depiction of the instrument and the status lamp are grayed out briefly during the restart. Afterwards, the status lamp lights up **orange** and the depiction of the instrument appears once again in color. Information on the start process is displayed in the status window. Once the restart is complete, the icon will reappear in color and the status lamp will light up **green**.

Regulate temperature

Target temperature sample holder	In this input field, enter the desired target temperature to which the sample holder is to be regulated. The entered temperature must be within the permissible range. The default value is 25 °C.

	Click this icon to start the temperature control on the sample holder. For this, the temperature defined in the **Target temperature sample holder** input field applies. **Note**: The temperature control at the sample vessel can not be started in this area.
	Click this icon to cancel the temperature control. **Note**: The temperature control at both the sample holder and the sample vessel can be stopped here.

See also

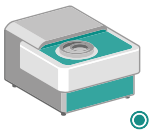
Instruments – Properties (chapter 5.12.2.5, page 865)

Spectrometer – Properties (chapter 5.12.2.10, page 871)

5.12.2.10.3 OMNIS NIR Analyzer Solid – Manual control

The following functions and information are displayed in the **Manual control** window for a reserved instrument of the **OMNIS NIR Analyzer Solid** type:

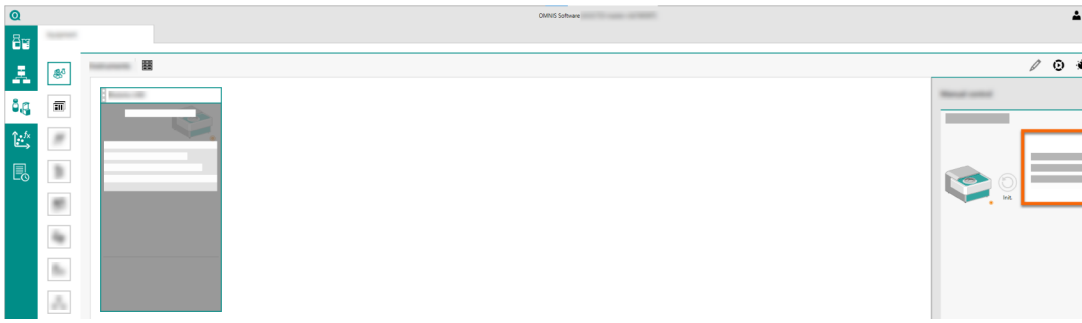
Status display



The depiction of the instrument and the color of the status lamp represent the status of the spectrometer: *Instrument status*.

Start process of the spectrometer

As soon as the spectrometer is switched on and the start process begins, the status window of the manual operation displays the status and the duration of the start process so far. The spectrometer cannot be operated during the start process. This may take up to 20 minutes.



Restart (Init.)

Click this icon to restart the spectrometer.

The icon, the depiction of the instrument and the status lamp are grayed out briefly during the restart. Afterwards, the status lamp lights up **orange** and the depiction of the instrument appears once again in color. The status window with the information on the start process is displayed. Once the restart is complete, the icon will reappear in color and the status lamp will light up **green**. The status window is hidden.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

Instruments – Manual control (chapter 5.12.2.6, page 867)

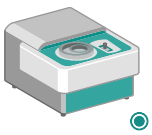
Instruments – Status (chapter 5.12.2.3, page 859)

Spectrometer – Properties (chapter 5.12.2.10, page 871)

5.12.2.10.4 OMNIS NIR Analyzer Liquid/Solid – Manual control

The following functions, parameters, and information are displayed in the **Manual control** window for a reserved instrument of the **OMNIS NIR Analyzer Liquid/Solid** type:

Status display and status window

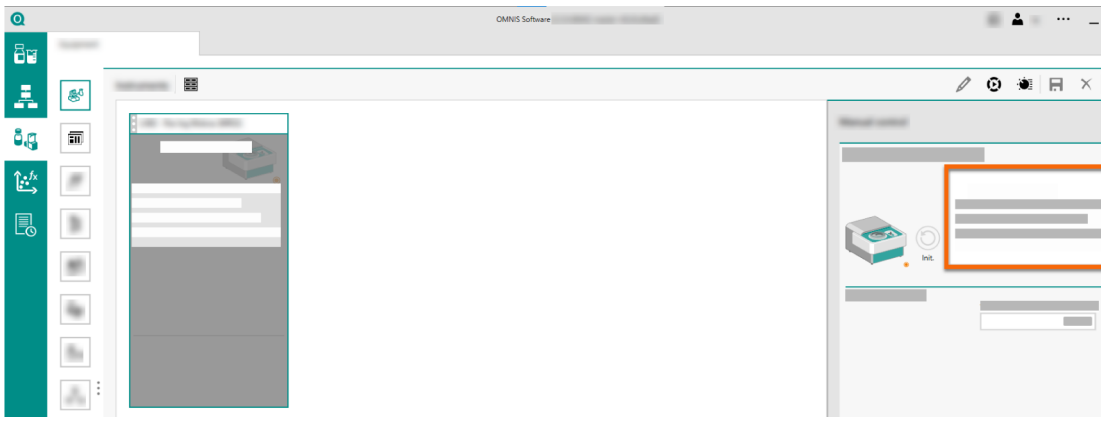


The depiction of the instrument and the color of the status lamp represent the status of the spectrometer: *Instrument status*. Additionally, the status and the duration of the start process is displayed in the status window, along with the following information:

Target temperature sample holder or **Target temperature sample vessel**	Depending on the setting, the temperature that is controlled on either the sample holder or the sample vessel is displayed.
Temperature sample holder or **Temperature sample vessel**	Depending on the setting, the temperature currently reached on either the sample holder or the sample vessel is displayed.

Start process of the spectrometer

As soon as the spectrometer is switched on and the start process begins, the status window of the manual operation displays the status and the duration of the start process so far. The spectrometer cannot be operated during the start process. This may take up to 20 minutes.



Restart (Init.)

	Click this icon to restart the spectrometer. The icon, the depiction of the instrument and the status lamp are grayed out briefly during the restart. Afterwards, the status lamp lights up **orange** and the depiction of the instrument appears once again in color. Information on the start process is displayed in the status window. Once the restart is complete, the icon will reappear in color and the status lamp will light up **green**.

Regulate temperature

Target temperature sample holder	In this input field, enter the desired target temperature to which the sample holder is to be regulated. The entered temperature must be within the permissible range. The default value is 25 °C.
	Click this icon to start the temperature control on the sample holder. For this, the temperature defined in the **Target temperature sample holder** input field applies. **Note**: The temperature control at the sample vessel can not be started in this area.
	Click this icon to cancel the temperature control. **Note**: The temperature control at both the sample holder and the sample vessel can be stopped here.

See also

Instruments – Properties (chapter 5.12.2.5, page 865)

Spectrometer – Properties (chapter 5.12.2.10, page 871)

5.12.2.11 Cubis II Balance – Properties

After selecting the **Cubis II Balance** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **Cubis II Balance** type in the **Specific data** subsection:

Balance data	
Manufacturer	Manufacturer of the balance.
Model	Model of the balance.
Instrument ID 1 **Instrument ID 2**	IDs that identify the balance. They can be changed in the device settings of the balance to allow for the balance to be localized and identified.
Package version	Firmware version that is installed on the balance.
Q-App Center version	Cubis Q-App Center version that is installed on the balance.

Connection	
IP address	Address of the instrument in the network.
TCP port	TCP port that is used for data transmission.

See also

Instruments – Properties (chapter 5.12.2.5, page 865)

Operating the Cubis II Balance (chapter 5.12.2.12.2, page 886)

5.12.2.12 Balance – Properties

After selecting the **Balance** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for the balance in the **Specific data** subsection:

Balance data	
Manufacturer	Manufacturer of the instrument. The entry is optional.
Model	Model of the balance. The entry is optional.
Instrument ID	Identifier that identifies the balance unambiguously. The entry is optional.

Connection configuration

The connection can be established via the RS-232 interface or the LAN interface (Ethernet). The selection and the entered parameters must match the settings of the balance. Depending on the selection, different input fields are displayed for the parameters.

Parameters for the RS-232 connection:

RS-232	
COM port	Serial interface on the PC to which the data is to be transferred (e.g. COM1).
Baud rate	Transfer rate.
Data bit	Number of data bits.
Parity	Type of parity testing.
Stop bit	Number of stop bits.
Handshake	Type of the data transfer protocol.
Maximum waiting time	Maximum waiting time for receiving an answer from the balance. As soon as this time is exceeded, the communication to the balance is interrupted. If a determination is being carried out at the same time, it is canceled due to the interruption of the communication.
Code page	Code page used for the data transmission.

Parameters for the Ethernet connection:

Ethernet	
IP address	Address of the instrument in the network. It must be written in a valid format: ▪ **IPv4**, e.g.: 192.0.2.235 ▪ **IPv6**, e.g.: 3ffe:1900:4545:3:200:f8ff:fe21:67cf
TCP port	TCP port that is used for data transmission.
Code page	Code page used for the data transmission.
Reconnect prior to command	With this check box, the connection to the balance can be re-established each time a command is sent. ▪ If the connection to the balance is lost multiple times (e.g. after another user tries to use the balance), this check box should be activated. ▪ If other users have problems connecting to the balance, the check box should not be activated. In general, it is not recommended for the balance to be used by multiple users simultaneously or alternately.

Protocol configuration

As protocol for the communication with a balance, an instruction set can be selected that is either pre-defined or user-defined. The selection and the entered parameters must match the settings of the balance.

- **SBI**: Control via parts of the **Sartorius Balance Interface** instruction set. Only the following weighing commands and tare commands are used:
  - **Weigh**: \1bP
  - **Tare**: \1bT
- **SICS**: Control via parts of the **Standard Interface Common Set** instruction set. Only the following weighing commands and tare commands are used:
  - **Weigh**: S
  - **Tare**: T
- **User-defined**: Control over a user-defined instruction set. If this protocol is selected, the following input fields for the parameters are displayed below:

User-defined	
Terminator for send	Terminator for sending in hexadecimal code (**\0D** = CR, **\0A** = LF). Consult the instructions for the balance for the corresponding terminator. ***Note***: Only leave this field empty if it is explicitly required for the protocol. Otherwise there can be problems with communication.
Terminator for receive	Terminator for receiving in hexadecimal code (**\0D** = CR, **\0A** = LF). Consult the instructions for the balance for the corresponding terminator.
Weigh	These command definitions are sent to the balance with the **WEIGH** command. Consult the instructions for the balance.

User-defined	
Weighing response pattern	Pattern which is looked for in the response of the balance to the weighing command that was sent. The sample is defined using regular expressions (RegEx). Additional information on regular expressions: *(see "RegEx – Regular expression", chapter 5.11.9.5.16, page 840)* It is possible to work with named capturing groups in the regular expressions. All of the appearances of a value can thus be found and consolidated in a group. After the definition of the capturing group, the corresponding RegEx expression must be entered. 3 capturing groups are relevant for the balance: ▪ **(?<value>)**: Weight, e.g. as numerical value with decimal places: **(?<value>\d+\.\d+)** ▪ **(?<unit>)**: Unit, e.g. for grams: **(?<unit>[g])** ▪ **(?<sign>)**: Algebraic sign (optional), e.g. for a positive or negative weight: **(?<sign>[+-]?)** Example of an entry for a positive or negative weight with decimal places in grams or milligrams: **(?<sign>[-+]?)[ ]*(?<value>\d*\.\d+)[ ]*(?<unit>[g|mg])** To ensure that only responses of the balance are taken into account, the entry can be written protocol-specific. Example for SICS: **[sS] [sS][ ]*(?<sign>[-+]?)[ ]*(?<value>\d*\.\d+)[ ]*(?<unit>[g|mg])** The field can also be left empty. In that case, the OMNIS Software interprets the response on its own.
Tare	The signs defined here are sent to the balance with the **TARE** command. Consult the instructions for the balance.
Tare response pattern	Pattern which is looked for in the response of the balance to the tare command that was sent. The pattern must either correspond to a RegEx expression or be empty. If the field is left empty, the software does not expect a response to the TARE command. *(see "RegEx – Regular expression", chapter 5.11.9.5.16, page 840)*

Once the connection protocol is selected, the connection test can be carried out with the **[Check connection]** button:

Connection test	
Use [Print] key	Carry out the connection test using the **[Print]** key. When pressing the **[Print]** key on the balance, the recorded weight is sent to the software.
Send weigh command	Carry out the connection test using a weigh command. A **WEIGH** command is sent to the balance and the recorded weight is sent as response to the software.

See also

Configuring the balance (chapter 5.12.2.12.1, page 884)

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.2.12.1 Configuring the balance

Balances of the **Cubis II** series from Sartorius come with automatic configuration and additional features. These are not described in this manual. Detailed instructions for connecting and operating devices of the **Cubis II Balance** type can be found here: *(see "Operating the Cubis II Balance", chapter 5.12.2.12.2, page 886)*

Prerequisites:

- The balance is connected to the computer via the RS-232-interface or via the local Ethernet network.

1 Displaying balances

- Click on to open the **Inventory** window in **Equipment** ▶ **Instruments**.
- Open the selection list with ⌄ and select the **Other instruments** subsection.

All the available instruments are displayed.

2 Assigning a balance

- Insert the desired instrument of the **Balance** type from the instrument list per drag and drop into the area on the right.

The balance can be configured.

3 Entering the properties of the balance

- Click on to open the **Properties** window.
- Open the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*
  - Enter the name for the balance in the **Product information** parameter group. This name is saved in the software. When a backup is created, the name is not transferred. In this parameter group, the product type of the balance can also be found.
  - The article number and the serial number can be entered in the **Production data** parameter group.

- Open the **Specific data** subsection: *(see "Cubis II Balance – Properties", chapter 5.12.2.11, page 880), (see "Balance – Properties", chapter 5.12.2.12, page 880)(see "Balance – Properties", chapter 5.12.2.12, page 880)*
  - The manufacturer, the model and the instrument ID for the balance can be entered in the **Balance data** parameter group.
  - Select the type of connection and configure the connection in the **Connection configuration** parameter group.
  - Select the desired transmission protocol in the **Protocol configuration** parameter group. For the **User-defined** option, you have to define the protocol yourself.

4 Checking the connection

- Click **[Check connection]**.
- Select the desired option:
  - **Use [Print] key**: For the connection test, the **[Print]** key must be pressed on the balance. Doing so will send the weight to the software.
  - **Send weigh command**: For the connection test, a **WEIGH** command is sent to the balance to request the weight.

If the connection has been established:

- If the data displayed is correct, click on **[Connection OK]**.
  The configuration is saved automatically. The status changes to **Ready** and the status light changes from orange to **green**.

If the connection could not be established:

- If no data is displayed or if the displayed values are not correct, click on **[Connection not OK]**.
  The configuration is not saved. The status changes to **not initialized** and the status light continues lighting up **orange**.
- Compare the settings on the balance with the connection configuration and the protocol configuration in the **Specific data** subsection and correct the parameters, if necessary.
- Run the connection test again.

The connection needs to be retested if the connection to the balance has been interrupted or the connection configuration or the protocol configuration of the balance has been changed.

See also

Balance – Properties (chapter 5.12.2.12, page 880)

Cubis II Balance – Properties (chapter 5.12.2.11, page 880)

Instruments – Properties (chapter 5.12.2.5, page 865)

Operating the Cubis II Balance (chapter 5.12.2.12.2, page 886)

WEIGH – Command variables (chapter 5.11.8.85.1, page 808)

WEIGH – Parameters (chapter 5.11.8.85, page 808)

5.12.2.12.2 Operating the Cubis II Balance

Weighing processes for an OMNIS system can be carried out with the **Cubis II Balance** from the balance series manufactured by the Sartorius company. To accomplish this, the respective application must first be installed on the balance via the Q-App Center. Please observe the corresponding instructions in the **Technical White Paper** in the *Metrohm Knowledge Base* on this.

These instructions describe the software-side connection and operation of the **Cubis II Balance**. The instrument manual for the balance can be found on the Sartorius website: *Sartorius website*

Connecting to the OMNIS system

In order to use the **Cubis II Balance**, first of all the balance must be connected with an OMNIS system. Proceed as follows:

Prerequisite:

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The **Cubis II Balance** is switched on, connected to the network via an Ethernet cable and in the same Ethernet network as the computer on which the OMNIS Software is running.
- The necessary installation steps corresponding to the instructions in the **Technical White Paper** have been carried out.
- In the OMNIS Software, the **Cubis II Balance** was assigned to the instrument area on the right-hand side under **Equipment** ▶ **Inventory** ▶ **Network instruments**.

If the user management for the OMNIS Software has been activated:

- The user who would like to use the balance with the OMNIS system has the right **Edit samples/not analyzed subsamples**.
- Either no user or the same user is logged on in the OMNIS system with which the balance is being used.

1 Selecting the OMNIS system

- On the display of the **Cubis II Balance**, select the computer name of the desired OMNIS-system.

The login window is displayed.

2 Logging in users

- Enter login information for the OMNIS system.

The balance is connected with the OMNIS system and the available work sequences are displayed.

All settings for the user management in the OMNIS Software also apply for working with the **Cubis II Balance**.

3 Selecting a workflow

- Select the desired work sequence.

Operating the Cubis II Balance

The selection of which work sequences are to be run with the OMNIS Software can be made on the **Cubis II Balance**:

- *Weighing in subsamples*: The weighing data for subsamples is recorded and entered in the sample list. The values for **Rack** and **Sample position** can be edited at this time.
- *Apply weighing data with REQUEST command*: During a determination, subsample data or variables are queried via a **REQUEST** command.
- *Control with OMNIS Software*: Control of the balance can be automated with the OMNIS Software.

Weighing in subsamples

Prerequisite:

- In the OMNIS Software there is a sample list with at least one subsample available for weigh-in. This subsample is in the **Ready** status and has an input field of the **Sample size** type which was defined in the subsample data of the operating procedure.

1 Selecting work sequences

- On the display, select the **Weigh in subsamples** work sequence.

All sample lists with at least one subsample available for weigh-in are displayed. They are sorted according to change date (most recently edited sample lists topmost).

If filtering of the data permissions is enabled, then only sample lists, samples, and subsamples with the data permissions of the user who is currently logged in will be listed.
Additional information on data permissions: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

2 Selecting a sample list

- Select the desired sample list in the display.

Once the sample list has been opened, all of the samples on the list are displayed with subsamples available for weigh-in.

The search function can be filtered directly for suitable sample lists.

3 Selecting a sample

- Select the desired sample in the display.

The search function can be filtered directly for suitable samples. A barcode reader can be used as the input instrument for the search.

The list includes all subsamples of the sample available for weigh-in. The following information is displayed for every subsample:

- Name of the subsample.
- Rack, that the sample is on, if this has been defined in the OMNIS Software.
- Sample position of the sample in the Rack, if this has been defined in the OMNIS Software.
- Sample size.
- Unit if this has been defined in the OMNIS Software.

4 Selecting a subsample

- On the display, select the desired subsample for weighing-in.

The search function can be filtered directly for suitable subsamples. A barcode reader can be used as the input instrument for the search.

The display for the weighing with the details for the specific subsample is opened. The following information is displayed for the subsample in this view:

- Name of the sample to which the subsample belongs.
  Name of the subsample.
- Position number of the subsample on the sample list.
- Sample size.
- Unit if this has been defined in the OMNIS Software.
- Rack that the subsample is on, if this has been defined in the OMNIS Software.
- Sample position of the subsample in the Rack, if this has been defined in the OMNIS Software.

- Minimum value and maximum value of the input field for the sample size if these have been defined in the OMNIS Software. During weighing, a graphical display shows whether the measured value is within the valid range between the minimum and maximum value. Only a valid value can be sent to the OMNIS Software.

If no unit for the sample size has yet been defined in the OMNIS Software, then this can be selected here by pressing on the unit. The units which are thereby available can be defined in the settings for the balance under the respective balance profile. If the unit has already been defined, then it can no longer be changed.

5 Weighing in a subsample

- Weigh the subsample on the balance and send the weight to the OMNIS Software via the orange **+** button.

If receipt of the weighing data is successful, then this will be signaled by a confirmation on the display. The confirmation disappears automatically as soon as the subsample is removed from the balance.

Should it not be possible to insert the weight and the unit into the input fields of the selected subsample, then an error message will appear.

Depending on the setting on the Q-App, either the list of the subsamples is displayed once again after the completion of the weighing-in, or the next subsample in the list is selected directly.

6 Optional: changing Rack and Sample position

The values for **Rack** and **Sample position** can be altered on the balance if these variables have been defined for the subsample. To accomplish this, click the respective specification in the sample list and change the respective value in the following display.

Apply weighing data with the REQUEST command

Prerequisite:

- The subsample must be in execution with a **REQUEST** command and the **REQUEST** pop-up window must be open.
- The subsample has an open input field of the **Sample size** type. The **REQUEST** command queries only the sample weight. Additional open subsample data must be queried separately, for which purpose a second **REQUEST** command is necessary.

If a **REQUEST** command is used with the **Cubis II Balance**, then 2 command parameters will not be observed:

- **Close pop-up window automatically**: The command is always closed automatically after data is received from the balance.
- **Minimum value** and **Maximum value**: The value entered is also sent to the OMNIS Software if it is not within the set limit values.

1 Selecting work sequences

- On the display, select the **Weighing-in via REQUEST** work sequence.

All open **REQUEST** commands are displayed. The following information is displayed for every **REQUEST**:

- Name of the associated sample.
- Name of the associated subsample.
- Operating procedure in which the command is located.

If multiple **REQUEST** commands are processed in a method, then the subsample must be updated after recording the weight so that the next command can be selected.

If filtering of the data permissions is enabled, then only sample lists, samples, and subsamples with the data permissions of the user who is currently logged in will be listed.
Additional information on data permissions: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

2 Selecting the REQUEST command

- Select the desired **REQUEST** command on the display.

The display for the weighing with the details for the **REQUEST** command that is being run is opened. The following information is displayed for the command in this view:

- Name of the associated sample.
- Name of the associated subsample.
- Name of operating procedure in which the command is located.
- Name of the method if the command is located in a method.
- Name of the command.
- Sample size.
- Unit if this has been defined in the OMNIS Software.

If the option **Edit unit** has been activated in the command or if the unit for the sample size has not yet been defined in the OMNIS Software, then it can be selected here.

3 Weighing in a subsample

- Weigh the subsample on the balance and send the weight to the OMNIS Software via the orange **+** button.

If the receipt of the weighing by difference data is successful, then this is shown by a confirmation on the display. The **REQUEST** command is closed on the OMNIS Software.

Should it not be possible to insert the weight and the unit into the input fields of the selected subsample, then an error message will appear.

Depending on the setting on the Q-App, either the list of the ongoing **REQUEST** commands is displayed once again after the completion of the command, or the next command in the list is selected directly.

Controlling with the OMNIS Software

Prerequisite:

- In the OMNIS Software there is a sample list with at least one subsample available for weigh-in. This subsample is in the **Ready** status and has an input field of the **Sample size** type which was defined in the subsample data of the operating procedure.

1 Selecting a work sequence

- On the display, select the **Control with OMNIS Software** work sequence.

The balance is now available only for commands of the **WEIGH** and **TARE** types which are being run in an ongoing operating procedure on the connected OMNIS system.

If filtering of the data permissions is enabled, then only sample lists, samples, and subsamples with the data permissions of the user who is currently logged in will be listed.
Additional information on data permissions: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

2 Using balances

- Use the balance on the OMNIS Software as usual:
  - **WEIGH**: The weight on the balance is queried.
  - **TARE**: Depending on the balance value, the balance is set to null (ZERO) or tared.

(see "Recording weighing data", chapter 5.10.7.4, page 280)

Behavior in the Audit Trail

If the Audit Trail for the OMNIS system is activated, then all actions via the application on the balance are recorded as follows:

- Every attempted login on the **Cubis II Balance** is recorded in an entry in the Audit Trail, including a reason for why it failed, if necessary.
- If a login is successful, then a further entry is made in the Audit Trail in which additional information regarding the balance is recorded:
  - Serial number of the balance
  - Host name of the balance which is used for all balance-specific entries for the system assignment
  - Display name of the balance in the OMNIS Software
  - Firmware version installed on the balance
  - Version of the Q-App installed on the balance with which the connection to the OMNIS Software was established
  - User logged in in the Q-App Center
  - Specification regarding the most recent calibration of the balance
- Every logout or every interruption of the connection between the OMNIS Software and the balance is recorded in an Audit Trail entry.
- The following information is recorded when a subsample is weighed in or weighed by difference:
  - Balance (host name) from which the balance value came
  - Memory ID which the value on the balance had
  - Specification regarding the validity of the calibration of the balance
  - Specification regarding the validity of the value

A weighed value is displayed as invalid in the Audit Trail if one of the following causes applies:

- The calibration of the balance is invalid (applies only with calibrated balances or if the "strict" safety level has been set on the balance).
- The balance has not been leveled (applies only with calibrated balances or if the "strict" safety level has been set on the balance).
- The balance has a negative gross value (applies only with calibrated balances).
- An error has occurred while using the **UserCal** Q-App.

When using the **Cubis II Balance** with a **WEIGH** command, the additional information regarding the weighing value is recorded on the sample list in the area **Subsample** in the **History** subsection:

- Memory ID under which the weighing data in the balance (on the alibi memory) was stored
- Specification regarding the validity of the calibration of the balance
- Specification regarding the validity of the calibration of the balance

See also

Balance – Properties (chapter 5.12.2.12, page 880)

Cubis II Balance – Properties (chapter 5.12.2.11, page 880)

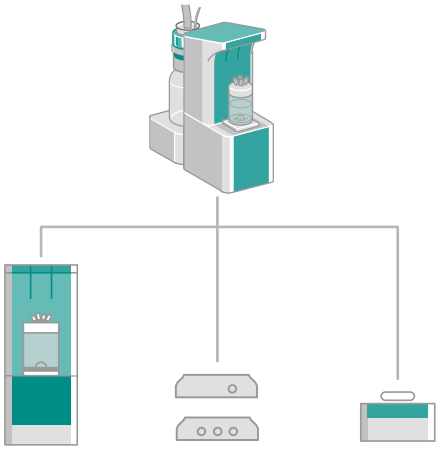
Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.3 Functional unit – Definition

A functional unit is a standalone component (such as a measuring module) of an instrument that can be used to execute commands. Functional units can be assigned to one or more work systems independently of one another. When a user reserves an instrument, all functional units of that instrument are available to that user for the creation of the work system.

Example: Titrator with four functional units

- Dosing unit
- digital measuring module
- analog measuring module
- Magnetic stirrer



See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Functional unit – Directory (chapter 5.12.3.1, page 894)

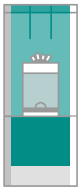
Functional unit – Manual control (chapter 5.12.3.5, page 906)

Functional unit – Status (chapter 5.12.3.2, page 904)

5.12.3.1 Functional unit – Directory

- *Functional units of OMNIS instruments*
- *Functional units of Metrohm USB instruments*
- *Functional units of other instruments*

Functional units of OMNIS instruments

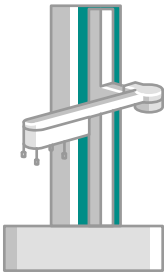
	2060 The NIR The functional unit can be used for near-infrared spectroscopic analysis in a process environment.
	**Dosing Drive** The functional unit is part of an **OMNIS Titrator**, **OMNIS Titration Module** or **OMNIS Dosing Module**. The **Dosing Drive** in combination with the **Cylinder Unit** attached is used as a dosing unit. The **Cylinder Unit** is equipped with a distributor with 4 ports and is available in various sizes.
	Gas Flow Unit The functional unit is included in the **Oven / Gas Flow Unit** of the oven module of a **OMNIS Sample Robot Oven**. The **Gas Flow Unit** is used to transport water vapor from the sample vessel into the KF titration cell by means of the carrier gas or air.

Liquid Sample Presentation

The functional unit is part of the instruments of the **OMNIS NIR Analyzer Liquid** and **OMNIS NIR Analyzer Liquid/Solid** types. The **Liquid Sample Presentation** is used for spectroscopic analysis of liquid samples.

Magnetic Stirrer

The functional unit can be part of the following instruments and modules: **OMNIS Coulometer**, **OMNIS Coulometer Module**, **OMNIS Dosing Module**, **OMNIS Main Module**, **OMNIS Titration Module**, **OMNIS Titrator**, **Oven Module** and **Pick&Place Module**.



Main Module Pick&Place

The functional unit is part of an **OMNIS Sample Robot** and is used to transport sample vessels on the sample robot.

Measuring Module Analog

The functional unit can be used in instruments of the **OMNIS Titrator** and **OMNIS Titration Module** type. The functional unit is used as a measuring module for analog sensors.

The following sensor types are available: Temperature sensor, pH electrode, metal electrode, polarizable metal electrode, ion-selective electrode and other sensor.

Measuring Module Conductivity

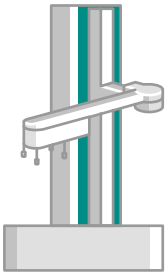
The functional unit can be used in instruments of the **OMNIS Titrator** and **OMNIS Titration Module** type. The functional unit is used as a measuring module for analog sensors of the conductivity measuring cell type.

Measuring Module Coulometry

The functional unit is installed in instruments of the **OMNIS Coulometer** and **OMNIS Coulometer Module** type. It consists of the **Coulometric Measuring Module** and the **Coulometric Generator**. Analog sensors of the polarizable metal electrode and temperature sensor types can be connected to the **Coulometric Measuring Module**. Generator electrodes can be connected to the **Coulometric Generator**.

Measuring Module Digital

The functional unit can be used in instruments of the **OMNIS Titrator** and **OMNIS Titration Module** type. The functional unit is used as a measuring module for digital sensors of the **dTrode** type. The following sensor types are available: pH electrode, metal electrode, ion-selective electrode, and Thermoprobe.

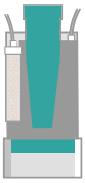


OMNIS Main Module

The functional unit is part of a **OMNIS Sample Robot**, **OMNIS Sample Robot NIR** and **OMNIS Sample Robot Oven** and is used to transport sample vessels between the sample racks and the workstations.

OMNIS Rod Stirrer

The functional unit can be connected to the MDL connector of an OMNIS instrument.

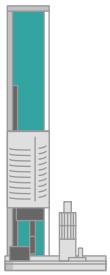


OMNIS Solvent Module

The functional unit can be controlled via the OMNIS Software or operated manually. The **OMNIS Solvent Module** is used for reliable addition of solvent and aspirating titration vessel content without contact with the reagents.

Oven Unit

The functional unit is installed in the **Oven / Gas Flow Unit** of the oven module of a **OMNIS Sample Robot Oven** and is used to heat the vial.



Oven Module

The functional unit is part of an **OMNIS Sample Robot Oven**. It has a turntable and a lift with which the vial is transported from the vial cradle to the oven for analysis and back again.

Peristaltic Pump

The functional unit is installed in the **Pump Module** of a **OMNIS Sample Robot** and can be used for various liquid handling tasks (e.g. aspiration or rinsing). A pump module is equipped with either 2 or 4 peristaltic pumps.

Pick&Place Module

The functional unit is part of an **OMNIS Sample Robot**. It contains a lift for moving the titration head vertically and a slide that can move the 2 beaker holders for sample beakers to defined positions.

The front beaker holder is used for the sample beakers, while the rear one can be used either for the rinsing beaker or for the storage beaker.

Solid Sample Presentation

The functional unit is part of the instruments of the **OMNIS NIR Analyzer Solid** and **OMNIS NIR Analyzer Liquid/Solid** types. This **Solid Sample Presentation** is used for the spectroscopic analysis of solid samples.

Functional units of Metrohm USB instruments

800 Dosino

The functional unit can be connected to the MSB connectors of Metrohm USB instruments. The **800 Dosino** with connected **807 Dosing Unit** is used as a buret.

The **807 Dosing Unit** is available in various sizes.

801 Stirrer

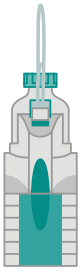
The functional unit can be connected to the MSB connectors of Metrohm USB instruments.

803 Ti Stand

The functional unit is connected to the MSB connectors of Metrohm USB instruments. The **803 Ti Stand** is used for volumetric or coulometric Karl Fischer titrations. With the installed pump, it is possible to aspirate the titrated solution manually and to add new solvent without having to open the titration cell.

804 Ti Stand

The functional unit is connected to the MSB connectors of Metrohm USB instruments. The **804 Ti Stand** is a controller for the rod stirrer **802 Stirrer**.



805 Dosimat

The functional unit can be connected to the MSB connectors of Metrohm USB instruments. The **805 Dosimat** with connected **806 Exchange Unit** is used as a buret.

The **806 Exchange Unit** is available in various sizes.

External Pump Socket

The functional unit is installed in the tower of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**. Depending on the instrument version, the tower features 0 to 2 pump connecters. The functional unit is used as a connector and for the operation of an external pump.

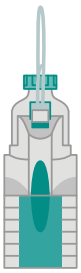
Gas Flow Unit

The functional unit is installed in the tower of instruments of the **874 Oven Sample Processor** type and is part of the **Oven / Gas Flow Unit**. The functional unit enables the transport of water vapor out of the sample vessel and into the KF titration cell with the aid of carrier gas or air.

Interface Coulometry

The functional unit is installed in instruments of the **851 Titrando** or **852 Titrando** types.

The functional unit is used as an interface for analog sensors and generator electrodes. The following sensor types are available: Temperature sensor and polarizable metal electrode.



Internal Dosing Drive

The functional unit is part of the following instruments: **888 Titrando**, **890 Titrando**, **904 Titrando** and **906 Titrando**. The **Internal Dosing Drive** with connected **806 Exchange Unit** is used as a buret.

The **806 Exchange Unit** is available in various sizes.

Measuring Interface Analog

The functional unit is installed in instruments of the **852 Titrando** type. The functional unit is used as a measuring interface for analog sensors.

The following sensor types are available: Temperature sensor and polarizable metal electrode.

Measuring Interface Analog

The functional unit is installed in instruments of the **890 Titrando** type. The functional unit is used as a measuring interface for analog sensors.

The following sensor type is available: polarizable metal electrode.

Measuring Interface Analog

The functional unit is installed in instruments of the **855 Robotic Titrosampler** type. The functional unit is used as a measuring interface for analog sensors.

The following sensor types are available: temperature sensor, pH electrode, metal electrode, polarizable metal electrode, ion-selective electrode and other electrode.

Measuring Interface Analog

The functional unit is installed in instruments of the **902 Titrando** type. The functional unit is used as a measuring interface for analog sensors.

The following sensor types are available: Temperature sensor, pH electrode, metal electrode, ion-selective electrode and other electrode.

Measuring Interface Analog

The functional unit is installed in instruments of the **867 pH Module**, **888 Titrando**, **901 Titrando**, **904 Titrando**, **905 Titrando**, **906 Titrando** and **907 Titrando** type. The functional unit is used as a measuring interface for analog sensors.

The following sensor types are available: temperature sensor, pH electrode, metal electrode, polarizable metal electrode, ion-selective electrode and other electrode.

Measuring Interface Conductivity

The functional unit is installed in instruments of the **856 Conductivity Module** type. The functional unit is used as a measuring interface for analog sensors of the conductivity measuring cell type.

Measuring Interface Analog + Measuring Interface iConnect

The functional unit consists of a **Measuring Interface Analog** to which a **Measuring Interface iConnect** is connected. The functional unit is installed in instruments of the **867 pH Module**, **888 Titrando**, **901 Titrando**, **904 Titrando**, **905 Titrando**, **906 Titrando** and **907 Titrando** type.

The **Measuring Interface iConnect** is used as a measuring interface for sensors of the **iTrode** type. The following sensor types are available: pH electrode and metal electrode.

Measuring Interface Analog + Measuring Interface iConnect

The functional unit consists of a **Measuring Interface Analog** to which a **Measuring Interface iConnect** is connected. The functional unit is installed in instruments of the **902 Titrando** type.

The **Measuring Interface iConnect** is used as a measuring interface for sensors of the **iTrode** type. The following sensor types are available: pH electrode and metal electrode.

Membrane Pump (Aspirate)

The functional unit is part of the tower of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**. Depending on the instrument version, the tower features 0 to 1 membrane pumps. The **Membrane Pump (Aspirate)** is used for aspirating liquid media.

Membrane Pump (Rinse)

The functional unit is part of the tower of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**. Depending on the instrument version, the tower features 0 to 1 membrane pumps. The **Membrane Pump (Rinse)** is used for pumping liquid media.

Oven Unit

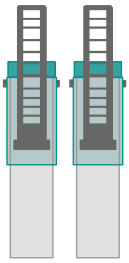
The functional unit is installed in instruments of the **874 Oven Sample Processor** type and is part of the **Oven / Gas Flow Unit**. The functional unit is used for software-controlled temperature control for heating the sample vessel.

Remote Box MSB

The functional unit can be connected to the MSB connectors of Metrohm USB instruments. The **Remote Box MSB** is used as interface for the connector of RS-232 devices (e.g. 849 Level Control) that can be controlled via remote lines.

Tower

The functional unit is part of the 1-tower version of the **814 USB Sample Processor**, the **815 Robotic USB Sample Processor XL** or the **855 Robotic Titrosampler**. The functional unit is comprised of the tower and the turntable and is used, together with the mounted **Sample Processor Rack**, for approaching sample vessels.

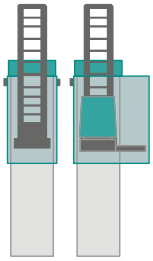


Tower

The functional unit is part of the 2-tower version of the **814 USB Sample Processor** or the **815 Robotic USB Sample Processor XL**. The functional unit is comprised of the towers and the turntable and is used, together with the mounted **Sample Processor Rack**, for approaching sample vessels.

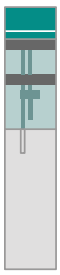
Tower + 786 Swing Head

The functional unit is part of the 1-tower version of the **814 USB Sample Processor**, the **815 Robotic USB Sample Processor XL** or the **855 Robotic Titrosampler** with **786 Swing Head** connected. The functional unit is comprised of the tower, the **786 Swing Head** and the turntable and is used, together with the mounted **Sample Processor Rack**, for approaching sample vessels at positions on the rack and at external positions.



Tower + 786 Swing Head

The functional unit is part of the 2-tower version of the **814 USB Sample Processor** or the **815 Robotic USB Sample Processor XL** with 1 to 2 **786 Swing Head** connected. The functional unit is comprised of the towers, the **786 Swing Head** and the turntable and is used, together with the mounted **Sample Processor Rack**, for approaching sample vessels at positions on the rack and at external positions.



Tower

The functional unit is comprised of the tower and the turntable of the **874 Oven Sample Processor** and is used, together with the mounted **Sample Processor Rack**, for approaching sample vessels.

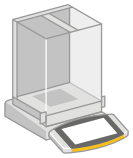
Tower Stirrer Socket

The functional unit is installed in the tower of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**. The functional unit is used as a connector and for the operation of an **802 Stirrer** or a **741 Magnetic Stirrer**.

Functional units of other instruments

Balance

The functional unit can be used for weighing in samples and for entering further sample data. The balance is connected to the OMNIS system via the RS-232 interface or the Ethernet network.



Cubis II Balance

The functional unit can be used for weighing in samples and for entering further sample data. The complete sequence of steps for weighing can be executed directly on the balance, if an instrument of the **Cubis II Balance** type from the balance series from Sartorius is used.

Serial Device

An instrument can be connected to the serial interface via RS-232 interface.

See also

Additional component – Directory (chapter 5.12.5.1, page 993)

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

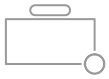
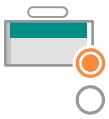
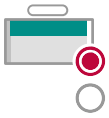
Functional unit – Manual control (chapter 5.12.3.5, page 906)

Functional unit – Status (chapter 5.12.3.2, page 904)

5.12.3.2 Functional unit – Status

The icons of the functional units are displayed differently, depending on their status. In addition, all functional units that can be actively actuated are equipped with a status light. The color and the condition of the status light varies, depending on the status of the functional unit.

The status of the functional units is represented as follows:

		The functional unit is not connected.
		The functional unit is ready for operation.
	(flashes 1/s)	The functional unit is in use.
		The functional unit must be initialized. Jamming may be present in a functional unit of the types **OMNIS Sample Robot**, **Sample Processor**, **Dosing Unit**, **800 Dosino**, **805 Dosimat** or **Internal Dosing Drive**. In case of jamming, this has to be fixed according to the instructions in the error messages displayed before the functional unit can be re-initialized.
	(flashes 1/s)	The functional unit is initializing.
	(flashes 3/s)	The functional unit is currently in the error state.

In addition to the status display, the icon shows that the functional unit is reserved.

	The functional unit belongs to a work system that is assigned to a method in the running determination.

Double-clicking on a connected functional unit opens the Manual control.

See also

Functional unit – Manual control (chapter 5.12.3.5, page 906)

Instruments – Status (chapter 5.12.2.3, page 859)

5.12.3.3 Assigning a functional unit to a command

As soon as one or more work systems have been assigned to a method, the appropriate functional units will be automatically assigned to the commands contained therein, insofar as these are present and unambiguous in the work system. Only the functional units for which their execution is feasible are available for each command. If more than one functional unit of the same type is contained in the work system, than automatic assignment of the functional units is not possible, and the functional unit must be assigned manually.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The method must be assigned a work system.
- The method is opened in which the functional units must be assigned manually to the commands.

1 Opening the command properties

- Select the desired command in the method editor.
- Click on to open the **Properties** window.
- Select the **Execute with** subsection.

2 Assigning functional unit manually

- Enable the check box next to the functional unit to assign it to the command.

3 Defining Solution conditions and Sensor conditions (optional)

Defining **Solution conditions** and **Sensor conditions** in accordance with the following instructions: *(see "Defining solution conditions and sensor conditions", chapter 5.12.7.4, page 1020)*

Depending on the command, **Solution conditions** and **Sensor conditions** can be defined when an intelligent solution or a digital sensor is used.

See also

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Method – Definition (chapter 5.11.3, page 413)

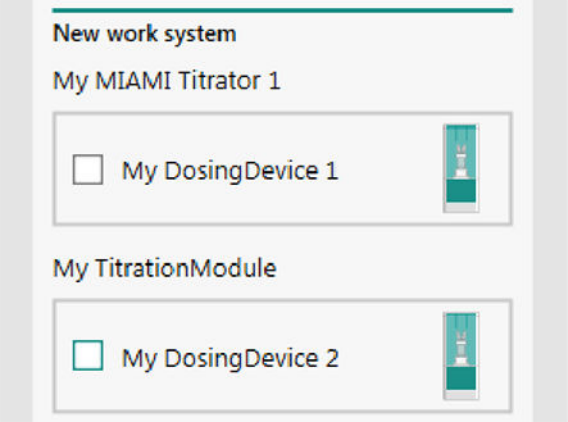
5.12.3.4 Removing assigned functional units from a command

1 Opening command properties

- Select the desired command in the method editor.
- Click on the icon to open the **Properties** window.
- Select the **Execute with** subsection.

2 Removing the functional unit

- Deactivate the check box next to the functional unit to remove it from the command.



See also

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Method – Definition (chapter 5.11.3, page 413)

5.12.3.5 Functional unit – Manual control

Manual control allows the functional units connected to the reserved instruments to be actuated directly, i.e. without defining a process (operating procedure, method), a sample and subsample. The prerequisites for this are:

- The associated instrument is switched on.
- The associated instrument is recognized by the OMNIS Software.
- The associated instrument is reserved under **Equipment** ► **Instruments**.
- The functional unit is not occupied by a process sequence.

Stirrers are an exception: During a determination in manual control, the stirring rate set in the **STIR** commands can be changed.

Opening the manual control

	Click this icon to open the **Manual control** of the selected functional unit. As an alternative, double-click the desired functional unit.

Functions

If the functional unit can be manually actuated, the functions for manual control and the associated settings are displayed in the **Manual control** window. In addition, measured values for ongoing actions and status messages are displayed here. Certain functional units (e.g. dosing unit or main module Pick&Place) can also be initialized manually.

Functions with icons

Click the following icons to execute the respective functions:

	Initialize functional unit.
	Start process.
	Stop process.
	Enable function.
	Disable function.
	Increase stirring rate.
	Reduce stirring rate.
	Enable **Park** function.

5.12.3.6 805 Dosimat – Properties

After selecting the **805 Dosimat** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for the 2 components **806 Exchange Unit** and **805 Dosimat** in the **Specific data** subsection:

806 Exchange Unit

Information on the exchange unit is displayed in the **Specific data** subsection. The use of the ports as well as further parameters can be modified.

Fill port	
Maximum filling rate	Enter the maximum permissible rate (in mL/min) for filling at the **Fill port**. For the **Maximum filling rate**, the following rule applies: **Maximum filling rate** = **3*cylinder volume**. In addition, the instrument verifies that this rate is not bigger than 3 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate. The **Maximum filling rate** has to be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.
Dosing port	
Maximum dosing rate	Enter the maximum permissible rate (in mL/min) for dosing at the **Dosing port**. For the **Maximum dosing rate**, the following rule applies: **Maximum dosing rate** = **3*cylinder volume**. In addition, the instrument verifies that this rate is not bigger than 3 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate. The **Maximum dosing rate** has to be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.
Preparation	
Volume	Enter the volume that is to be dosed during the preparation process. We recommend entering the volume of the cylinder used for the preparation.
Cycles	Enter the number of cycles with which the preparation process is to be run.
Cylinder	
Cylinder volume	Display the volume of the cylinder installed in the exchange unit.
Article number	Display the number that unambiguously identifies the cylinder.
Serial number	Display the serial number of the cylinder.

805 Dosimat

Information on the dosing drive is displayed in the **Specific data** subsection.

Connector	
MSB connector	Display the number of the MSB connector on the Metrohm USB device that the functional unit is connected to.

See also

800 Dosino – Manual control (chapter 5.12.3.10, page 920)

805 Dosimat – Manual control (chapter 5.12.3.9, page 917)

Dosing unit – Manual control (chapter 5.12.3.11, page 925)

Instruments – Directory (chapter 5.12.2.2, page 854)

Instruments – Properties (chapter 5.12.2.5, page 865)

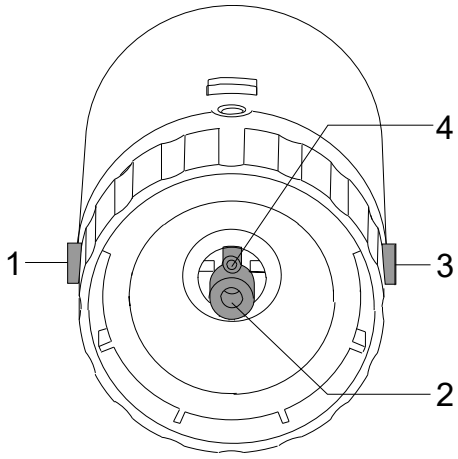
5.12.3.7 Dosing device (MSB) – Properties

After selecting the **800 Dosino** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for the 2 components **807 Dosing Unit** and **800 Dosino** (dosing drive) in the **Specific data** subsection:

807 Dosing Unit

The **807 Dosing Unit** is equipped with a distributor with 4 ports. The ports are used in the following way by default:



1	**Port 1** Dosing port 1	**2**	**Port 2** Fill port
3	**Port 3** Dosing port 2	**4**	**Port 4** Special port

Information on the dosing unit is displayed in the **Specific data** subsection. The use of the ports as well as further parameters of the dosing unit can be modified.

Fill port	**Port via which the dosing unit is filled.**
Port assignment	Assigns the desired port as **Fill port**.
Tubing length	Length of the tubing (in cm) that is connected to the fill port of the dosing unit. If no tubing is connected, a **Tubing length** of **0** must be entered in order to prevent automatic preparation via this port.
Tubing diameter	Inner diameter of the tubing (in mm), that is connected to the **Fill port** of the dosing unit.
Maximum filling rate	Maximum permissible rate (in mL/min), used for filling at **Fill port**. For the **Maximum filling rate**, the following rule applies: **Maximum filling rate** = **10/3*cylinder volume** In addition, the instrument checks whether this rate is greater than 10/3 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate. The **Maximum filling rate** must be reduced if viscous solutions are aspirated or if tubing thinner than the standard tubing is used.

Dosing port 1	**Dosing port 1 for dosing with the dosing unit by default.**
Port assignment	Assigns the desired port as **Dosing port 1**.

Dosing port 1	**Dosing port 1 for dosing with the dosing unit by default.**
Tubing length	Length of the tubing that (in cm) that is connected to dosing port 1 of the dosing unit. If no tubing is connected, a **Tubing length** of **0** must be entered in order to prevent automatic preparation via this port.
Tubing diameter	Inner diameter of the tubing (in mm), that is connected to the **Dosing port 1** of the dosing unit.
Maximum dosing rate	Maximum permissible rate (in mL/min), used for dosing at the **Dosing port 1**. For the **Maximum dosing rate**, the following rule applies: **Maximum dosing rate** = **10/3*cylinder volume** In addition, the instrument checks whether this rate is greater than 10/3 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate. The **Maximum dosing rate** must be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.
Dosing port 2	**Dosing port 2 that can be used for dosing with the dosing unit.**
Port assignment	Assigns the desired port as **Dosing port 2**.
Tubing length	Length of the tubing that (in cm) that is connected to dosing port 2 of the dosing unit. If no tubing is connected, a **Tubing length** of **0** must be entered in order to prevent automatic preparation via this port.
Tubing diameter	Inner diameter of the tubing (in mm), that is connected to the **Dosing port 2** of the dosing unit.
Maximum dosing rate	Maximum permissible rate used for dosing at the **Dosing port 2**. For the **Maximum dosing rate**, the following rule applies: **Maximum dosing rate** = **10/3*cylinder volume** In addition, the instrument checks whether this rate is greater than 10/3 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate. The **Maximum dosing rate** must be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.
Special port	**Port for special tasks (e.g. for aspirating air or ejecting residual liquids during the rinsing procedure).**
Port assignment	Assigns the desired port as **Special port**.
Tubing length	Length of the tubing (in cm) that is connected to the special port of the dosing unit. If no tubing is connected, a **Tubing length** of **0** cm must be entered in order to prevent automatic preparation via this port.

Special port	**Port for special tasks (e.g. for aspirating air or ejecting residual liquids during the rinsing procedure).**
Tubing diameter	Inner diameter of the tubing (in mm), that is connected to the **Special port** of the dosing unit.
Maximum rate	Maximum permissible rate (in mL/min) for dosing or aspirating at the **Special port**. For the **maximum rate**, the following rule applies: **Maximum rate** = **10/3*cylinder volume** In addition, the instrument checks whether this rate is greater than 10/3 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate.

Effect of the tubing parameters on the volume
The two parameters **Tubing length** and **Tubing diameter** for the connection tubing at the ports of the dosing unit enable the OMNIS Software to automatically calculate the required volume for preparation and emptying. Preparation or emptying is executed with the **Preparing** function or the **Empty** function in the manual control of the dosing unit.

Valve	**Parameters for moving the valve on the distributor**
Valve disk rotation direction	Rotation direction of the valve disk to reach the required port: ▪ **Ascending** Rotate to target port in ascending port number order. ▪ **Descending** Rotate to target port in descending port number order. ▪ **Automatic** Rotate to target port via shortest path. ▪ **Do not rotate over**: If this option is selected, then the following specific parameter is displayed: – **Do not rotate over**
Do not rotate over	Selection of the port that is not to be traversed when the valve disk is rotated. In this way, contamination caused by dripping is avoided.

Cylinder	**Information on the glass cylinder in the dosing unit.**
Cylinder volume	Volume of the cylinder inserted in the dosing unit.
Article number	Number that identifies the cylinder unambiguously.
Serial number	Serial number of the cylinder.

800 Dosino

Information on the dosing drive is displayed in the **Specific data** subsection.

Connector	
MSB connector	Number of the MSB connector on the Metrohm USB instrument that the functional unit is connected to.

See also

800 Dosino – Manual control (chapter 5.12.3.10, page 920)

805 Dosimat – Manual control (chapter 5.12.3.9, page 917)

Dosing unit – Manual control (chapter 5.12.3.11, page 925)

Instruments – Directory (chapter 5.12.2.2, page 854)

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.3.8 Dosing unit (OMNIS) – Properties

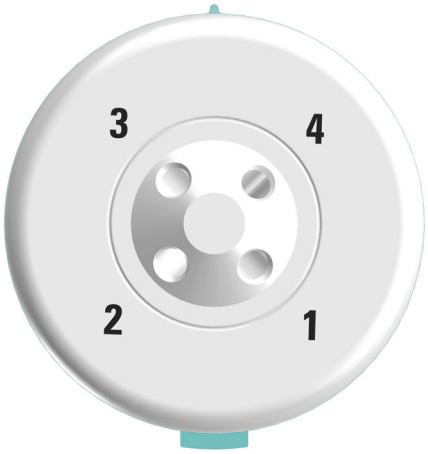
After selecting the **Dosing Unit** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for the **Cylinder Unit** in the **Specific data** subsection:

No data is displayed for the **Dosing Drive**.

Cylinder Unit

The **cylinder unit** used in the dosing unit is equipped with a distributor with 4 ports. The ports are used in the following way by default:



1	**Port 1** Dosing port 1	**2**	**Port 2** Fill port
3	**Port 3** Dosing port 2	**4**	**Port 4** Special port

Information on the cylinder unit is displayed in the **Specific data** subsection. The port assignment as well as further parameters of the cylinder unit can be modified.

Fill port	**Port via which the cylinder unit is filled by default.**
Port assignment	Assigns the desired port as **Fill port**.
Tubing length	Length of the tubing that is connected to the fill port of the cylinder unit (in cm). If no tubing is connected, a **Tubing length** of **0** must be entered.
Tubing diameter	Inner diameter of the tubing that is connected to the fill port of the cylinder unit (in mm).
Maximum filling rate	Maximum permissible rate for filling. In addition, the instrument checks whether this rate is greater than 6 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate. The **Maximum filling rate** must be reduced if air bubbles arise when aspirating the solution.
Dosing port 1	Dosing port 1 for dosing with the cylinder unit by default.
Port assignment	Assigns the desired port as **Dosing port 1**.

Tubing length	Length of the tubing that is connected to dosing port 1 of the cylinder unit (in cm). If no tubing is connected, a **Tubing length** of **0** must be entered.
Tubing diameter	Inner diameter of the tubing that is connected to dosing port 1 of the cylinder unit (in mm).
Maximum dosing rate	Maximum permissible rate for dosing. In addition, the instrument checks whether this rate is greater than 6 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate. The **Maximum dosing rate** must be reduced if highly viscous solutions are dosed or if tubing thinner than the standard tubing is used.

The maximum dosing rate and the port assignment of **Dosing port 1** are used when the dosing unit is initialized. If no cylinder unit was put in place or detected, then initialization will take place at a third of the maximum possible speed.

Dosing port 2	**Dosing port 2 that can be used for dosing with the cylinder unit.**
Port assignment	Assigns the desired port as **Dosing port 2**.
Tubing length	Length of the tubing that is connected to dosing port 2 of the cylinder unit (in cm). If no tubing is connected, a **Tubing length** of **0** must be entered.
Tubing diameter	Inner diameter of the tubing that is connected to dosing port 2 of the cylinder unit (in mm).
Maximum dosing rate	Maximum permissible rate for dosing. In addition, the instrument checks whether this rate is greater than 6 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate. The **Maximum dosing rate** must be reduced if highly viscous solutions are dosed or if tubing thinner than the standard tubing is used.

Special port	**Port for special tasks (e.g. for aspirating air or ejecting residual liquids during the rinsing procedure).**
Port assignment	Assigns the desired port as **Special port**.
Tubing length	Length of the tubing that is connected to the special port of the cylinder unit (in cm). If no tubing is connected, a **Tubing length** of **0** must be entered.
Tubing diameter	Inner diameter of the tubing that is connected to the special port of the cylinder unit (in mm).
Maximum rate	Maximum permissible rate for dosing or aspirating at the special port. In addition, the instrument checks whether this rate is greater than 6 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate.

Effect of the tubing parameters on the volume

The two parameters **Tubing length** and **Tubing diameter** for the connection tubing at the ports of the cylinder unit enable the OMNIS Software to automatically calculate the required volume for preparation and emptying. Preparation or emptying is initiated with the **Preparing** function or the **Empty** function in the manual control of the cylinder unit.

Valve	**Parameters for moving the valve on the distributor**
Valve disk rotation direction	Rotation direction of the valve disk opening to reach the required port: ▪ **Ascending** Rotate to target port in ascending port number order. ▪ **Descending** Rotate to target port in descending port number order. ▪ **Automatic** Rotate to target port via shortest path. ▪ **Do not rotate over**: If this option is selected, then the following specific parameter is displayed: – **Do not rotate over**
Do not rotate over	Selection of the port that is not to be traversed when the valve disk is rotated. In this way, contamination caused by dripping is avoided.

Cylinder	**Information on the glass cylinder in the cylinder unit.**
Cylinder volume	Volume of the cylinder installed in the cylinder unit.
Article number	Number that identifies the cylinder unambiguously.
Serial number	Serial number of the cylinder.

Service	
Last buret calibration	Date on which the last buret calibration was carried out.
Result of the buret calibration	Shows the result of the buret calibration: ▪ **Not yet executed** The calibration has not been carried out yet. ▪ **Passed** The calibration was carried out successfully. ▪ **Failed** The calibration was not successful.

See also

800 Dosino – Manual control (chapter 5.12.3.10, page 920)

805 Dosimat – Manual control (chapter 5.12.3.9, page 917)

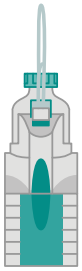
Dosing unit – Manual control (chapter 5.12.3.11, page 925)

Instruments – Directory (chapter 5.12.2.2, page 854)

5.12.3.9 805 Dosimat – Manual control

If a functional unit of the **805 Dosimat** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit appear in the **Manual control** window.

Status display



The current status of the dosing device is visible in the icon display. Additionally, the following information is displayed in the status window:

- Current level of volume that has been pumped with the executed function.
- Function being carried out (**Dosing volume…**, or **Filling volume…**)

Initializing

	Click on this icon to initialize the buret. During the initialization, the status symbol of the buret flashes **orange**. As soon as initialization of the dosing device is complete, the status symbol lights up **green**.

Functions

Preparing

This function is used in the following situations:

- Removing air bubbles from the exchange unit or the tubing.
- Putting the exchange unit back into operation after an extended standstill.

To avoid precipitation or carry-over in the exchange unit when changing solutions, the exchange unit must be disassembled and cleaned according to the instructions in the *Product manual (chapter 5.1.1)*.

Function	Activate the **Preparing** function. The number of cycles for the **Preparing** function and the volume to be dosed during preparation can be defined in the parameter group **Preparation** under **Properties** ▶ **Specific data**.
	Click this icon to start the **Preparing** function. In the process, the parameters defined for the exchange unit will be used.
	Click this icon to cancel the process.

Fluid may escape when preparing the exchange unit. To avoid this, proceed as follows:

- Make sure that all buret tips are pointing into a provided container.
- Confirm the warning message to proceed with the process.

Dosing

Dosing volume	Volume that is dosed.
	Click this icon to start dosing.
	Click this icon to cancel the process.
Dosing rate	Rate at which the solution is dosed. Depending on the cylinder volume, it may not be possible to reach the specified dosing rate. If **Maximum** is selected, then the highest possible dosing rate is used for dosing. If air bubbles are created when aspirating the solution, the dosing rate needs to be reduced. This can occur if highly viscous solutions are dosed or if tubing thinner than the standard tubing is used.
Filling rate	Rate at which the cylinder is filled after the specified volume of solution has been dosed. The filling rate must be reduced if air bubbles are created when aspirating the solution. This can occur if highly viscous solutions are dosed or if tubing thinner than the standard tubing is used.

Filling

Filling rate	Rate at which the dosing unit is filled. The filling rate must be reduced if air bubbles are created when aspirating the solution. This can occur if highly viscous solutions are dosed or if tubing thinner than the standard tubing is used.
	Click this icon to fill the cylinder.
	Click this icon to cancel the process.

See also

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.3.10 800 Dosino – Manual control

If an instrument of the **800 Dosino** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the instrument appear in the **Manual control** window.

Status display

The current status of the buret is visible in the icon display. Additionally, the following information is displayed in the status window:

- Name of the solution that the buret is attached to.
- Used port.
- Current level of volume that has been pumped with the executed function.
- Function being carried out (**Dosing volume…**, **Filling volume…** or **Aspirating volume…**)

Initializing

Click on this icon to initialize the buret (**800 Dosino** with **807 Dosing Unit**).

During the initialization, the status symbol of the buret flashes **orange**. As soon as initialization is complete, the status symbol lights up **green**.

Functions

Preparing

This function is used in the following situations:

- Removing air bubbles from the **807 Dosing Unit** or the connected tubing.
- Putting the system back into operation after an extended standstill.

To avoid precipitation or carry-over when changing the solution, intermediate flushing can be carried out using the **Preparing** function:

- Empty the buret using the **Empty** function.
- Select the **Preparing** function.
- Immerse the filling tube in a bottle of water and click ▶.
- Empty the buret using the **Empty** function.
- After completing the preparation sequence, attach the buret to the second solution and click ▶ again.

Function	Activate the **Preparing** function.
▶	Click this icon to start the **Preparing** function. In the process, the parameters defined for the buret will be used.
■	Click this icon to cancel the process.

Fluid may escape when preparing the buret. To avoid this, proceed as follows:

- Make sure that all buret tips are pointing into a provided container.
- Confirm the warning message to proceed with the process.

Empty

This function is used in the following situations:

- Empty the buret used.
- Flush and change to a new solution.
- Prepare the system for an extended standstill.

Function	Activate the **Empty** function.
▶	Click this icon to start the **Empty** function. In the process, the parameters defined for the buret will be used.
■	Click this icon to cancel the process.

To empty, remove the buret from the bottle. Fluid may escape when emptying the buret. To avoid this, proceed as follows:

- Make sure that all buret tips are pointing into a provided container.
- Confirm the warning message to proceed with the process.

Dosing

Dosing mode	Selection of the command with which the defined volume is to be dosed: ▪ **ADD**: Dosing with automatic compensation of the mechanical clearance of the dosing piston. ▪ **DOSE**: Dosing without automatic compensation of the mechanical clearance of the dosing piston. If **DOSE** is selected, the following specific parameters appear: – **Dosing port** – **Fill port**
Dosing volume	Volume to be dosed.
	Click this icon to start dosing.
	Click this icon to cancel the process.
Dosing rate	Rate at which the solution is to be dosed. Depending on the cylinder volume, it may not be possible to reach the specified dosing rate. If **Maximum** is selected, then the highest possible dosing rate is used for dosing. The **Dosing rate** has to be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.
Dosing port (only for DOSE)	Port that is to be used to dose the specified volume. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**

Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening should be moved.
Filling rate	Rate at which the cylinder is to be filled after the specified volume of solution has been dosed. The **Filling rate** has to be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.
Fill port (only for DOSE)	Port that is to be used for filling the cylinder. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening should be moved.

Filling

Filling mode	Selection of the command with which the cylinder is to be dosed: ▪ **FILL**: Filling with automatic compensation of the mechanical clearance of the dosing piston. – **Filling rate** – **Fill port** ▪ **ASPIRATE**: Aspiration without automatic compensation of the mechanical clearance of the dosing piston. If **ASPIRATE** is selected, the following specific parameters appear: – **Aspiration rate** – **Aspiration volume** – **Aspiration port**

Filling rate or **Aspiration rate**	Rate at which the buret is to be filled or the volume is to be aspirated. The **Filling rate** or **Aspiration rate** has to be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.
Aspiration volume (only for ASPIRATE)	Volume to be aspirated.
Fill port or **Aspiration port**	Port via which the cylinder is to filled or the volume is to be aspirated. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1** (only for **ASPIRATE**): Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2** (only for **ASPIRATE**): Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening should be moved.
	Click this icon to fill the cylinder.
	Click this icon to stop the process. With the **800 Dosino**, filling cannot be canceled immediately. The process is stopped as soon as the cylinder is completely full.

See also

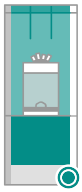
Instruments – Properties (chapter 5.12.2.5, page 865)

Operating the 800 Dosino (chapter 5.12.3.12, page 931)

5.12.3.11 Dosing unit – Manual control

If a functional unit of the **Dosing Unit** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit appear in the **Manual control** window.

Status display



The current status of the dosing unit is visible in the icon display. Additionally, the following information is displayed in the status window:

- Name of the solution that is connected to the dosing unit.
- Used port.
- Current level of volume that has been pumped with the executed function.
- Function being carried out (**Dosing volume…**, **Filling volume…** or **Aspirating volume…**)

Initialize

	Click this icon to initialize the dosing unit. During initialization, the status symbol of the dosing unit flashes **orange**. As soon as initialization is complete, the status symbol lights up **green**. The status display on the instrument shows the alternating status at the same time. During initialization, the dosing piston is moved to a specific position. During this process, liquid can be dosed if a cylinder unit is attached. The initialization can also be run without an attached cylinder unit. Initializing is necessary if the dosing drive has lost its saved initialization position (e.g. if the instrument has been switched off during operation) or if the dosing unit is jammed.

For a dosing unit that has not been initialized, only the functions **Initialize** and **Exchange position** are available in manual control. The cylinder unit can be removed (e.g. to remove jamming) in the **Exchange position**.

Functions

Preparing

This function is used in the following situations:

- Removing air bubbles from the dosing unit or the connected tubing.
- Putting the system back into operation after an extended standstill.

To avoid precipitation or carry-over when changing the solution, intermediate flushing can be carried out using the **Preparing** function:

- Empty the dosing unit using the **Empty** function.
- Select the **Preparing** function.
- Immerse the filling tube in a bottle of water and click .
- Empty the dosing unit using the **Empty** function.
- After completing the preparation sequence, attach the bottle cap of the dosing unit to the second solution and click again.

Function	Enable the **Preparing** function.
	Click this icon to start the **Preparing** function. In the process, the parameters defined for the dosing unit will be used.
	Click this icon to cancel the process.

Liquid can escape when preparing the dosing unit. To avoid this, proceed as follows:

- Check if all buret tips are pointing into a provided vessel.
- Confirm the warning message to proceed with the process.

Empty

This function is used in the following situations:

- Empty the dosing unit used.
- Flush and change to a new solution.
- Prepare the system for an extended standstill.

Function	Enable the **Empty** function.
	Click this icon to start the **Empty** function. In the process, the parameters defined for the dosing unit will be used.
	Click this icon to cancel the process.

To empty, remove the dosing unit from the bottle. Liquid can escape when emptying the dosing unit. To avoid this, proceed as follows:

- Check if all buret tips are pointing into a provided vessel.
- Confirm the warning message to proceed with the process.

Exchange position

This function is used in the following situations:

- Removing the cylinder unit, e.g. for exchanging.

Before starting the **Exchange position** function, execute the **Empty** function. This ensures that liquids are no longer in the cylinder unit.

Function	Enable the **Exchange position** function.
	Click this icon to start the **Exchange position** function. In the process, the parameters defined for the dosing unit will be used.
	Click this icon to cancel the process.

Dosing

Dosing mode	Selection of the command with which the defined volume is to be dosed: ▪ **ADD**: Dosing with automatic compensation of the mechanical clearance of the dosing piston. ▪ **DOSE**: Dosing without automatic compensation of the mechanical clearance of the dosing piston. If **DOSE** is selected, then the following specific parameter appears: – **Fill port**
Dosing volume	Volume to be dosed.
Dosing rate	Rate at which the solution is to be dosed. Depending on the cylinder volume, it may not be possible to reach the specified dosing rate. If **Maximum** is selected, then the highest possible dosing rate is used for dosing. The **Dosing rate** has to be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.

Dosing port	Port that is to be used to dose the defined volume. ▪ **ADD**: Dosing with automatic compensation of the mechanical clearance of the dosing piston. – **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. – **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **DOSE**: Dosing without automatic compensation of the mechanical clearance of the dosing piston. – **Fill port**: Port that is defined in the specific data of the functional unit as fill port. – **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. – **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. – **Special port**: Port that is defined in the specific data of the functional unit as special port. – **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening is to be moved.
Filling rate	Rate at which the cylinder is filled after the specified volume of solution has been dosed. The **Filling rate** has to be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.

Fill port	Port that is to be used for filling the cylinder. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening is to be moved.
	Click this icon to start dosing.
	Click this icon to cancel the process.

Filling

Filling mode	Selection of the command with which the cylinder is to be dosed: ▪ **FILL**: Filling with automatic compensation of the mechanical clearance of the dosing piston. If **FILL** is selected, the following specific parameters appear: – **Fill level** – **Filling rate** – **Fill port** ▪ **ASPIRATE**: Aspiration without automatic compensation of the mechanical clearance of the dosing piston. If **ASPIRATE** is selected, then the following specific parameters appear: – **Aspiration volume** – **Aspiration rate** – **Aspiration port** – **Dispensing rate** – **Dispensing port**

Fill level	Volume to which the cylinder is to be filled. If the cylinder is already partly filled, then only the difference in volume will be added. With **Maximum**, it will be filled up to the maximum possible fill level of the cylinder unit used.
Aspiration volume	Volume to be aspirated.
Filling rate or **Aspiration rate**	Rate at which the dosing unit is to be filled or the volume is to be aspirated. The **Filling rate** or **Aspiration rate** has to be reduced if viscous solutions are dosed or if tubing thinner than the standard tubing is used.
Fill port or **Aspiration port** (for ASPIRATE additionally Dosing port 1 and Dosing port 2)	Port via which the cylinder is to filled or the volume is to be aspirated. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening is to be moved.
Dispensing rate	Rate at which the liquid is to be dispensed. If, in the **Equipment** work area, a **Maximum dosing rate** is defined for the selected port of the functional unit used that is smaller than the **Dispensing rate**, then the maximum dosing rate will be used. In addition, the instrument checks during dosing that this rate does not exceed the maximum permitted rate for the functional unit used. If this should be the case, then the instrument will reduce the rate. If viscous solutions are aspirated or if tubing is used that is thinner than standard tubing, then the rate needs to be reduced accordingly so that the dosing drive is not overloaded.

Dispensing port	Port via which the liquid is to be dispensed. ▪ **Fill port**: Port that is defined in the specific data of the functional unit as fill port. ▪ **Dosing port 1**: Port that is defined in the specific data of the functional unit as dosing port 1. ▪ **Dosing port 2**: Port that is defined in the specific data of the functional unit as dosing port 2. ▪ **Special port**: Port that is defined in the specific data of the functional unit as special port. ▪ **Absolute**: Selection of an absolute port position. If **Absolute** is selected, the following specific parameter is displayed: – **Absolute port position**
Absolute port position	Select the absolute port position (**Port 1–4**), to which the valve disk opening is to be moved.
	Click this icon to fill the cylinder.
	Click this icon to cancel the process.

See also

805 Dosimat – Properties (chapter 5.12.3.6, page 907)

Dosing device (MSB) – Properties (chapter 5.12.3.7, page 909)

Dosing unit (OMNIS) – Properties (chapter 5.12.3.8, page 913)

Functional unit – Status (chapter 5.12.3.2, page 904)

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.3.12 Operating the 800 Dosino

The OMNIS Software can be used to execute the following actions for the **800 Dosino** and the connected **807 Dosing Unit**:

- *(see "Operating the 800 Dosino", chapter 5.12.3.12, page 931)*
  This function is required to remove **800 Dosino** from the **807 Dosing Unit** if an error has occurred while dosing.
- *(see "Emptying and cleaning the 807 Dosing Unit", page 933)*
  The function is required to empty the **807 Dosing Unit**, e.g. for a solution change or before a prolonged downtime.
- *(see "Preparing the 807 Dosing Unit", page 934)*
  The function is required for each new start-up or if the **807 Dosing Unit** is to be used after prolonged downtime.

- *(see "Changing a solution", page 935)*
  The function is required if **807 Dosing Unit** is to be used with another solution.

Further information on the functions described here can be found in the *800 Dosino* and *807 Dosing Unit* manuals.

Changing the dosing unit after an error

Prerequisite:

- The instrument to which the **800 Dosino** is connected has been reserved in the OMNIS Software under **Equipment** ▶ **Inventory** ▶ **Network instruments**.
- The **800 Dosino** set up on **807 Dosing Unit** is mounted on a bottle.
- The port display on **807 Dosing Unit** does not show **2**.
- The overview of the instrument under **Equipment** ▶ **Instruments** is open.
- The status display of the **800 Dosino** is permanently lit in **green**.

1 Opening the manual control window

- Click on to open the **Manual control** window.
  or
- Double-click on the **800 Dosino** functional unit to open the **Manual control** window.

2 Filling or emptying the dosing unit

- In the **Fill** section, fill the dosing unit by clicking on .
  or
- In section **Functions**, select the **Empty** function from the selection list.
- Click on to start the function.

The flat stopcock is then rotated automatically to the exchange position.

The port display on **807 Dosing Unit** shows **2**.

3 Removing the tubing

- Remove the tubing from the dosing port and any other ports.

The dosing unit can now be removed from the bottle.

Emptying and cleaning the 807 Dosing Unit

Prerequisite:

- All buret tips always point into vessels to catch escaping solution.
- The instrument to which the **800 Dosino** is connected has been reserved in the OMNIS Software under **Equipment** ▶ **Inventory** ▶ **Network instruments**.
- The **800 Dosino** set up on **807 Dosing Unit** is mounted on a bottle.
- The overview of the instrument under **Equipment** ▶ **Instruments** is open.
- The status display of the **800 Dosino** is permanently lit in **green**.

1 Opening the manual control

- Click on to open the **Manual control** window.
  or
- Double-click on the **800 Dosino** functional unit to open the **Manual control** window.

2 Emptying the dosing unit

- In section **Functions**, select the **Empty** function from the selection list.
- Click on to start the function.
- Observe the warning and click on **[Execute]** to confirm.

The dosing unit is emptied completely.

3 Removing the tubing

- Remove the tubing on the dosing port. If other ports besides the dosing port and the fill port are occupied by hoses, then these must also be removed.

4 Removing the dosing unit

- Unscrew the **807 Dosing Unit** from the bottle.

5 Fastening the tubing

- Immerse the tubing attached to the fill port in a bottle with water.
- Attach tubing to the dosing port and insert the buret tip into a container.

6 Rinsing the 807 Dosing Unit

- In section **Functions**, select the **Preparing** function from the selection list.
- Click on ▶ to start the function.
- Observe the warning and click on **[Execute]** to confirm.
- Select the **Empty** function.
- Click on ▶ to start the function.
- Observe the warning and click on **[Execute]** to confirm.

The rinsing process can be repeated if necessary.

The **807 Dosing Unit** can now be unscrewed from **800 Dosino** and set aside.

Preparing the 807 Dosing Unit

Prerequisite:

- The instrument to which the **800 Dosino** is connected has been reserved in the OMNIS Software under **Equipment** ▶ **Inventory** ▶ **Network instruments**.
- The overview of the instrument under **Equipment** ▶ **Instruments** is open.
- The status display of the **800 Dosino** is permanently lit in **green**.

1 Screwing the dosing unit onto the solution

- Attach tubing to the fill port.
- Screw the **807 Dosing Unit** onto the desired solution.
- Attach tubing to the dosing port and insert the buret tip into a container.
- Connect the **800 Dosino** to the **807 Dosing Unit**.

Make sure that all buret tips always point into vessels to catch escaping solution.

2 Opening the manual control

- Click on ⏵ to open the **Manual control** window.
  or
- Double-click on the **800 Dosino** functional unit to open the **Manual control** window.

3 Rinsing the 807 Dosing Unit

- In section **Functions**, select the **Preparing** function from the selection list.
- Click on ▶ to start the function.
- Observe the warning and click on **[Execute]** to confirm.
- Select the **Empty** function.
- Click on ▶ to start the function.
- Observe the warning and click on **[Execute]** to confirm.

The rinsing process can be repeated if necessary.

The **800 Dosino** and **807 Dosing Unit** are now ready for operation.

Changing a solution

Prerequisite:

- All buret tips always point into vessels to catch escaping solution.
- The instrument to which the **800 Dosino** is connected has been reserved in the OMNIS Software under **Equipment** ▶ **Inventory** ▶ **Network instruments**.
- The **800 Dosino** set up on **807 Dosing Unit** is mounted on a bottle.
- The overview of the instrument under **Equipment** ▶ **Instruments** is open.
- The status display of the **800 Dosino** is permanently lit in **green**.

1 Opening the manual control

- Click on ▶ to open the **Manual control** window.
  or
- Double-click on the **800 Dosino** functional unit to open the **Manual control** window.

2 Removing the 807 Dosing Unit from the bottle

- In section **Functions**, select the **Empty** function from the selection list.
- Click on ▶ to start the function.
- Observe the warning and click on **[Execute]** to confirm.
- Unscrew the **807 Dosing Unit** from the bottle.

3 Attaching the 807 Dosing Unit to a new bottle

- Attach the **807 Dosing Unit** on the desired bottle.

- Click on ▶ to start the **Empty** function.
- Observe the warning and click on **[Execute]** to confirm.

If there is a possibility of precipitation or chemical reactions occurring when old and new solutions are mixed, then an interim rinse with an inert solvent is to be recommended.

4 Rinsing the 807 Dosing Unit

- In section **Functions**, select the **Preparing** function from the selection list.
- Click on ▶ to start the function.
- Observe the warning and click on **[Execute]** to confirm.
- Select the **Empty** function.
- Click on ▶ to start the function.
- Observe the warning and click on **[Execute]** to confirm.
- In section **Functions**, select the **Preparing** function from the selection list.
- Click on ▶ to start the function.
- Observe the warning and click on **[Execute]** to confirm.

The rinsing process can be repeated if necessary.
This step serves to avoid precipitation or carry-over when changing solutions in the dosing unit.

The bottle can now be used.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

Instruments – Directory (chapter 5.12.2.2, page 854)

Reserving and releasing instruments (chapter 5.12.2.4, page 861)

5.12.3.13 Rinsing the cylinder unit automatically

If solutions that crystallize quickly are used in a titration, this may cause damage to the cylinder unit used. In order to automatically rinse the cylinder unit at the end of the titration before prolonged non-use, Metrohm recommends including a corresponding method in the operating procedure.

In these instructions, 2 variants are described to create a corresponding method:

- *Downloading a method as a template and using it directly*
- *Creating a method yourself*

Downloading a method as a template and using it directly

Prerequisite:

- The user is familiar with the method creation according to the following instructions: *(see "Creating and editing a method", chapter 5.11.3.3, page 418)*
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Downloading the template

- Download the templates from the *Metrohm Knowledge Base*.
- Import the **Exchange position OMNIS dosing cylinder.opro** method into the OMNIS Software according to the instructions. *(see "Importing the templates", chapter 3.2, page 11)*

The **Exchange position OMNIS dosing cylinder.opro** method is located inside the ZIP file in the following directory: **OP templates** ▶ **Automation** ▶ **Liquid handling**.
Alternatively to this method, the **Clean and store cylinder unit.opro** operating procedure from the **OP templates** ▶ **Automation** ▶ **Best Practice OMNIS Cylinder units** directory can be used.

2 Using methods

- Check the parameters of the commands contained in the method and adjust them if necessary.
- Insert the method into an existing operating procedure at a suitable position. *(see "Creating and editing an operating procedure", chapter 5.11.1.3, page 387)*

Metrohm recommends inserting the method as the last step after titration.

Creating a method yourself

Prerequisite:

- The user is familiar with the method creation according to the following instructions: *(see "Creating and editing a method", chapter 5.11.3.3, page 418)*

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Creating a new method

- Create a new method or open an existing method in **Processes** ▶ **Methods**. *(see "Creating and editing a method", chapter 5.11.3.3, page 418)*
- Insert the following commands in the method in this order:
  - VALVE POS
  - PISTON POS
  - VALVE POS

2 Parameterizing the first VALVE POS command

- Define the command parameters in **Properties** ▶ **Parameters**:
- Select the **Absolute** option in the **Target position** field.
- Select the **Port 2** option in the **Absolute port position** field.

3 Parameterizing the PISTON POS command

- Define the command parameters in **Properties** ▶ **Parameters**:
- Enter a value in the **Target position** field between **0.00000** and **1.00000**.
- Select the **Formula** option in the **Flow rate** field.
- In the formula editor, create a formula according to the following scheme:
  Case('**CylinderVolume.CurrentCylinderUnit**.**Move piston to position 1**'**>0**;'**MaxFlowRate.Tube.FillPort.CurrentCylinderUnit**.**Move piston to position 1**';**300;300**). *(see "Case – Condition", chapter 5.11.9.5.2, page 834)*, *(see "PISTON POS – Command variables", chapter 5.11.8.42.1, page 732)*

4 Parameterizing the second VALVE POS command

- Define the command parameters in **Properties** ▶ **Parameters**:
- Select the **Absolute** option in the **Target position** field.
- Select the **Port 2** option in the **Absolute port position** field.

5 Saving a method

- Save the method by clicking on .

6 Using methods

- Insert the method into an existing operating procedure at a suitable position. *(see "Creating and editing an operating procedure", chapter 5.11.1.3, page 387)*

Metrohm recommends inserting the method as the last step after titration if the cylinder unit is not to be used for a prolonged period of time.

If the method is to be executed only under certain conditions, it can be inserted into a **IF** command. Additional information on the **IF** command: *(see "IF – Parameters", chapter 5.11.8.70, page 782)*

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Creating a work system (chapter 5.12.4.4, page 989)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

5.12.3.14 Executing tandem dosing

With tandem dosing, continuous and uninterrupted dosing can be carried out. Dosing is executed with 2 dosing devices in combination, so that one dosing device can be filled while the other dosing device carries out the dosing.

To ensure uninterrupted dosing, the following steps must be followed when configuring the tandem dosing:

1 Keeping filling times short

- Use the value **Maximum** in the **Filling rate** command parameter to keep the filling times short. The **Maximum filling rate** is used which has been defined in the **Equipment** work area for the functional unit used for the fill port. The viscosity and the density of the liquid must be taken into account.

2 Using 2 cylinders of the same size

- Use 2 cylinders with the same cylinder volume for tandem dosing. This prevents the cylinder units of both assigned dosing devices from having to be filled at the same time.
- If 2 cylinders of unequal size must be used (cylinder 2 > cylinder 1), the filling rate and the dosing rate of both cylinders must be adjusted in the properties of the functional units:
  Filling rate for the larger cylinder 2 ≧ dosing rate for the smaller cylinder 1 • ($V_{cylinder\ 2}$ / $V_{cylinder\ 1}$)

3 Keeping the filling rate higher than the dosing rate

- To ensure uninterrupted dosing, the filling rate must be higher than the dosing rate. The dosing rate must not exceed 75% of the value of the filling rate.

Carrying out tandem dosing

Prerequisite:

- A method with a **STAT pH** command or a **STAT U** command was created.
- A work system with at least 2 dosing devices is assigned to the method.

1 Assigning the dosing device

- Select the STAT command within the method.
- Click on to open the **Properties** window.
- Select a dosing device that is to be used for the dosing in **Properties** ▶ **Execute with**.

2 Activating tandem dosing

- Enable the **Tandem dosing** check box underneath the assigned dosing device.
- Select the desired other dosing device for the dosing in the **Secondary dosing device** selection list.

The dosing device that was selected first is the primary dosing device, the other is the secondary dosing device. The control (loading the method, starting the dosing etc.) is done via the primary dosing device.

Tandem dosing is activated. The determination can be started in the sample list. Both of the dosing devices carry out the dosing in combination during the determination.

See also

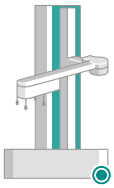
STAT – Principle (chapter 5.11.8.7, page 533)

STAT – Run (chapter 5.11.8.7.2, page 543)

5.12.3.15 Main module – Manual control

If a functional unit of the **Main Module Pick&Place** or **OMNIS Main Module** type is selected in the **Instruments** subsection, then the possible functions and parameters for the functional unit will appear in the **Manual control** window.

Status display

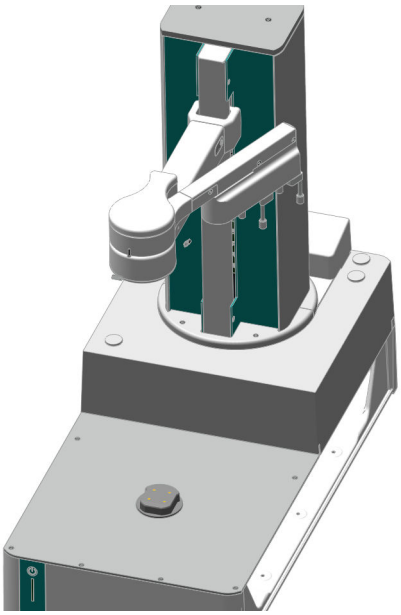


The depiction and the color of the status lamp represent the current status of the main module: *Functional units status*.

Initializing

	Click this icon to initialize the main module. During initialization, the status lamp of the main module flashes **orange**. As soon as the initialization is complete, the status lamp lights up **green**. If initialization is not possible, then the main module must be moved manually into park position.

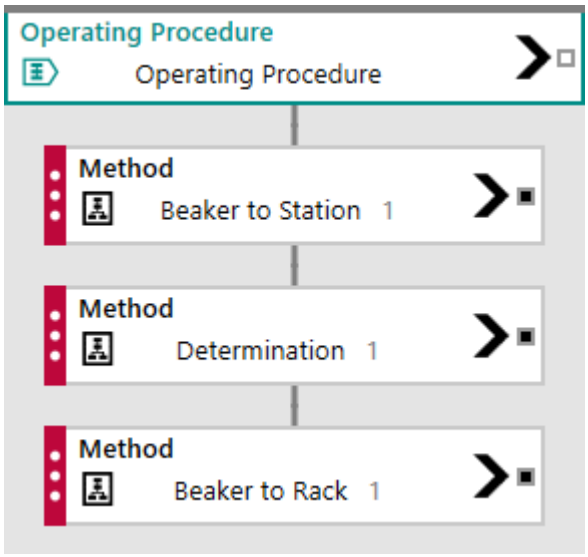
Parking the robot arm



P	Click this icon to move the robot arm into park position. This ensures safe access to the working area during ongoing operation (e.g. to exchange racks). The operating procedures running for the analysis pause as soon as the robot arm is no longer required by running methods. The robot arm moves into park position. A message indicates that the park position has been reached and the access is safe. The parking procedure can be interrupted at any time. Once the action has been completed (e.g. after a rack change), the robot arm is available once again for further determinations.

A rack that is used in the determination run and that is marked with the icon may not be replaced. One or more samples of this rack are still in progress and must be placed back onto the rack.

To keep the waiting time until parking short, it is useful to create a separate method for the determination and to separate this from the methods for transporting the vessel:



See also

Gas Flow Unit – Manual control (chapter 5.12.3.19.2, page 955)

OMNIS NIR Analyzer Liquid – Manual control (chapter 5.12.2.10.2, page 874)

OMNIS NIR Analyzer Liquid/Solid – Manual control (chapter 5.12.2.10.4, page 877)

OMNIS NIR Analyzer Solid – Manual control (chapter 5.12.2.10.3, page 876)

Oven Module – Manual control (chapter 5.12.3.18.1, page 949)

Oven Unit – Manual control (chapter 5.12.3.19.1, page 954)

Pick&Place Module – Manual control (chapter 5.12.3.20.1, page 956)

Pump module – Manual control (chapter 5.12.3.27, page 966)

5.12.3.16 Measuring interface – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **Interface** type in the subsection **Specific data**:

Specific data

Position	
Input	Display the position of the measuring input on the instrument.

Only applies to the Measuring interface analog:
Depending on the type of the measuring interface, a connector for a functional unit of the **Measuring Interface iConnect** type is available. If a **Measuring Interface iConnect** is connected, the properties of this functional unit are displayed above the properties of the **Measuring Interface Analog**.

See also

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.3.17 Measuring module – Manual control

If a functional unit of the **Measuring Module Analog**, **Measuring Module Digital**, **Measuring Module Conductivity** or **Measuring Module Coulometry** type is selected in the **Instruments** subsection, then the available functions, parameters, and information for the functional unit appear in the **Manual control** window. Different functions and parameters are displayed, depending on the product type.

Status display

The current status of the measuring module is visible in the instrument symbol display. Additionally, the following information is displayed in the status window:

- **Measured value**
- **Drift**
- **Temperature** (is not displayed if **Temperature** is selected as the measured quantity)

Measuring

Table 7 General functions

	Click this icon to start the measurement.
	Click this icon to cancel the measurement. After cancellation, the values last measured for **Measured value**, **Drift**, and, if applicable, **Temperature** are displayed in the status window.

Measuring Module Analog

Measured quantity	Selecting the measured quantity: ▪ **pH** ▪ **Potential U** ▪ **Potential U(I(pol))** ▪ **Temperature** ▪ **Concentration** The following parameter will also appear if **Potential U(I(pol))** is selected as the measured quantity: – **I(pol) DC**
Sensor name	Selection of the analog sensor that is to be used at the measuring input. If the default value **No sensor** is selected, then the measurement is canceled with an error.

Measuring input	Selection of the measuring input. ▪ **For measured quantities pH**, **Potential U**, **Concentration**: A **pH electrode**, an **ion-selective electrode**, a **metal electrode** or **another sensor** can be connected to **INPUT 1** or **INPUT 2**. ▪ **For measured quantity Potential U(I(pol))**: The polarizable metal electrode can be connected only to **INPUT 1**. ▪ **For measured quantity Temperature**: A temperature sensor, a pH electrode with an integrated temperature sensor or an ion-selective electrode with an integrated temperature sensor can be connected to **INPUT 1** or **INPUT 2**.
Temperature sensor (not available with measured quantity **Temperature**)	Selection of the sensor to be used to measure the temperature. **For measured quantities pH**, **Potential U** or **Concentration**: A temperature sensor, a pH electrode with an integrated temperature sensor or an ion-selective electrode with an integrated temperature sensor. If the default value **No temperature sensor** is selected, then the value is applied that was entered under **Temperature**. **Note**: For sensors with an integrated temperature sensor (pH electrodes, ion-selective electrodes), both measuring inputs must be set to **INPUT 1**.
Measuring input (not available with measured quantity **Temperature**)	Selection of the measuring input for temperature measurement. **Note**: If **Potential U(I(pol))** is selected as the measured quantity, then the temperature measurement can be taken only at **INPUT 2**. This means the selection cannot be edited.
Temperature (not available with measured quantity **Temperature**)	Enter the temperature that was measured with the external temperature sensor.

I(pol) DC	Enter the polarization current that is applied to the polarizable metal electrode during voltametric measurement. **Note**: Metrohm recommends entering the current in increments of 0.5 µA.

Measuring Module Digital

Measured quantity	Selecting the measured quantity: ▪ **pH** ▪ **Potential U** ▪ **Temperature** ▪ **Concentration**
Temperature (not available with measured quantity **Temperature**)	Enter the temperature that was measured with the external temperature sensor.

Measuring Module Conductivity

Measured quantity	Selecting the measured quantity: ▪ **Conductivity κ**
Sensor name	Selection of the conductivity measuring cell that is to be used at the measuring input. If the default value **No sensor** is selected, then the measurement is canceled with an error.
Temperature	Enter the temperature that was measured with the external temperature sensor.
Temperature compensation	Selection of the type of temperature compensation. ▪ **Constant factor**: If **Constant factor** is selected, then the following parameters will also appear: – **Reference temperature** – **Temperature coefficient** ▪ **DIN EN 27888**: If **DIN EN 27888** is selected, then the following parameter will also appear: – **Reference temperature** ▪ **No temperature compensation**

Reference temperature	Electrical conductivity depends greatly on temperature. The conductivity measured at a particular temperature is automatically converted to the conductivity of this reference temperature (usually 20 °C or 25 °C).
Temperature coefficient	Temperature compensation is carried out with the constant factor entered.

Measuring Module Coulometry

Measured quantity	Selecting the measured quantity: ▪ **Potential U(I(pol))** ▪ **Temperature** The following parameter will also appear if **Potential U(I(pol))** is selected as the measured quantity: – **I(pol) DC**
Sensor name	Selection of the analog sensor that is to be used at the measuring input. If the default value **No sensor** is selected, then the analysis is canceled with an error.
Measuring input	Indication only takes place at **INPUT 1**, while the temperature measurement can be taken only at **INPUT 2**. ▪ **For measured quantity Potential U(I(pol))**: The polarizable metal electrode can be connected only to **INPUT 1**. ▪ **For measured quantity Temperature**: A temperature sensor can be connected to **INPUT 1** or **INPUT 2**.
Temperature sensor (not available with measured quantity **Temperature**)	Selection of the sensor of type **Temperature sensor**, which is to be used to measure the temperature. If the default value **No temperature sensor** is selected, then the value is applied that was entered under **Temperature**.

Measuring input (not available with measured quantity **Temperature**)	Measuring input for temperature measurement. As the temperature measurement can be made only at **INPUT 2** with measured quantity **Potential U(I(pol))**, the selection cannot be edited.
Temperature (not available with measured quantity **Temperature**)	Enter the temperature that was measured with the external temperature sensor.
I(pol) DC	Enter the polarization current that is applied to the polarizable electrode during voltametric measurement. **Note**: Metrohm recommends entering the current in increments of 0.5 µA.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

5.12.3.18 Oven Module – Properties

After selecting the **Oven Module** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **Oven Module** type in the **Specific data** subsection:

Specific data

All positions	
Change height	Enter the height to which the oven module lift is to be moved in order to transport the vial between the handover position and the analysis position without collision.

Specific positions	
Work height for handover	Enter the height to which the oven module lift is to be moved if the turntable is in the handover position. The vial is transferred from the lift to the turntable at this height after the analysis. Once a value for the **Work height for handover** is entered, it is automatically adopted as **Special height for analysis** when the field is exited.
Work height for analysis	Enter the height to which the oven module lift is to be moved if the turntable is in the analysis position. The vial is in the oven at this height, and the septum piercing needle and the outlet needle have pierced through the septum. The analysis can be started.
Special height for analysis	Display the height that the oven module lift will move to if the turntable is in the analysis position. The transfer of the vial from the turntable to the lift is initiated at this height. The **Special height for analysis** corresponds to the **Work height for handover**.
Work height for conditioning	Enter the height to which the oven module lift is to be moved if the turntable is in the conditioning position. The septum piercing needle and the outlet needle have pierced through the septum at this height and are located in the conditioning tube. The system can be conditioned.

See also

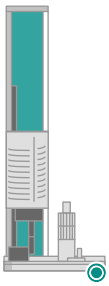
Assigning the lift height (chapter 5.12.3.18.2, page 952)

Oven Module – Manual control (chapter 5.12.3.18.1, page 949)

5.12.3.18.1 Oven Module – Manual control

If a functional unit of the **Oven Module** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit will appear in the **Manual control** window.

Status display



The current status of the oven module is visible in the icon display. In addition, the following information is displayed in the status window:

- Lift height
- Turntable position

Initializing

	Click on this icon to initialize the oven module. The lift of the oven module is initialized first, followed by the turntable. During initialization, the status display of the oven module flashes **orange**. Once the initialization of the oven module is complete, the status display lights up **green**.

Moving the lift

Target height	Select a defined height to which the lift is to be moved: ▪ **Work height**: Height that is defined in the properties of the oven module for a specific turntable position as the work height. ▪ **Change height**: Height that is defined in the properties of the oven module for all turntable positions as the change height. ▪ **Special height**: Height that is defined in the properties of the oven module for the analysis position of the turntable as the special height. It corresponds to the work height of the handover position. ▪ **Enter height**: Entry of an absolute height to which the lift is to be moved. If **Enter height** is selected, then the following parameter will also appear: – **Lift height** **Note**: If substitute values are selected, then the lift will use the specific lift height that is defined for the turntable position in which the turntable is when the command is executed. Additional information on assigning lift heights: *(see "Assigning the lift height", chapter 5.12.3.18.2, page 952)*.
Lift height	Enter the height (in mm) to which the lift is to be moved. A lift height of 0 mm corresponds thereby to the home position at the top end stop of the lift. If the **Assign lift heights** user right is available, then the **Assign current height** button will appear. Click on this button to assign the current lift height to a defined turntable position. The button is disabled if the turntable is not in one of the predefined positions.
	Click this icon to move the lift to the selected or entered lift height.
	Click this icon to cancel the process.
Lift rate	Speed at which the lift is to be moved.

Rotating the turntable

Target position	Select the position on the turntable to which it is to be rotated: ▪ **Handover position**: The vial cradle is located under the vial holder. ▪ **Analysis position**: The recess at the turntable is located under the vial holder. ▪ **Conditioning position**: The conditioning tube is located under the vial holder. This position may be activated only if the vial holder does not contain a vial.
	Click this icon to rotate the turntable to the selected target position.
	Click this icon to cancel the process.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

Oven Module – Properties (chapter 5.12.3.18, page 948)

5.12.3.18.2 Assigning the lift height

Predefined lift heights can be used for the positions on the turntable of the oven module of instruments of the **OMNIS Sample Robot Oven** type. The lift heights defined according to these instructions can be used as substitute values for the target height in the **LIFT** command and in the manual control.

The following lift heights can be defined for the turntable positions of the oven module:

- **Work height**: The work height depends on the turntable position:
  - Handover position
  - Analysis position
  - Conditioning position
- **Change height**: The change height is defined once and for all and applies to all turntable positions.

Note: The **Special height** at the analysis position corresponds value-wise to the work height at the handover position and can therefore be defined only in connection with this.

Prerequisite:

- The user has the **Assign lift heights** right.

1 Opening the manual control

- Select the **Oven Module** functional unit under **Equipment ► Instruments**. Double-click on the functional unit or click on to open the **Manual control** window.

2 Moving to the turntable position

- Select a turntable position and move to it under **Rotate turntable ► Target position**.

3 Moving to the lift height

- Select from the **Enter height** selection list under **Move lift ► Target height**.
- Move to the required lift height by entering the **Lift height** (in mm) in the input field.

4 Saving the lift height as a predefined height

- Click on **[Assign current height]** to open the **Assign lift height** dialog in which the current turntable position and the current lift height are displayed.
- Select the predefined height to which the current lift height is to be assigned under **Assign to**.
- Click on **[Assign]** to save the current lift height as the predefined height.

See also

Defining the lift height (chapter 5.12.3.30.3, page 978)

LIFT – Properties (chapter 5.11.8.48, page 738)

Oven Module – Manual control (chapter 5.12.3.18.1, page 949)

Sample rack – Properties (chapter 5.12.8.2, page 1025)

5.12.3.19 Oven / Gas Flow Unit – Properties

After selecting the **Oven Unit** functional unit, clicking on opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information for functional units of the **Oven / Gas Flow Unit** type (part of a **Oven Unit**) are available in the **Specific data** subsection:

No data is displayed for the **Gas Flow Unit**.

Specific data

Oven data	
Temperature correction	Enter the correction value for the measured temperature.
(only Oven Unit of 874 Oven Sample Processor)	The temperature of the oven unit is corrected by this value. This makes it possible to compensate for temperature differences between the oven temperature and the temperature on the interior of the oven.

The functional units **Oven Unit** and **Gas Flow Unit** are called **Oven / Gas Flow Unit** by default.
In order to clearly distinguish between the functional units, we recommend to change the product names accordingly.

See also

FLOW – Properties (chapter 5.11.8.60, page 758)

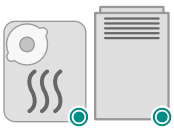
KFT – Properties (chapter 5.11.8.10.1, page 568)

TEMP – Properties (chapter 5.11.8.61, page 759)

5.12.3.19.1 Oven Unit – Manual control

If a functional unit of the **Oven Unit** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit will appear in the **Manual control** window.

Status display



The current status of the oven is visible in the icon display. In addition, the following information is displayed in the status window:

- Target temperature
- Temperature

Heating

	Click on this icon to heat the oven to the entered target temperature.
	Click this icon to cancel the process.

Target temperature	Temperature to which the oven is to be heated.

See also

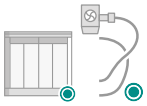
Functional unit – Status (chapter 5.12.3.2, page 904)

Oven / Gas Flow Unit – Properties (chapter 5.12.3.19, page 953)

5.12.3.19.2 Gas Flow Unit – Manual control

If a functional unit of the **Gas Flow Unit** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit will appear in the **Manual control** window.

Status display



The current status of the gas flow unit is visible in the icon display. In addition, the following information is displayed in the status window:

- Flow rate

Operating

	The gas flow unit is switched off. Click the switch to turn on the gas flow.
	The gas flow unit is switched on and runs until it is switched back off. Click the switch to turn the gas flow off.
Carrier gas inlet	Selection of the carrier gas inlet: ▪ **Pump** ▪ **Valve**
Flow rate	Flow rate of the carrier gas. Input range: 10– 150 mL/min
Carrier gas	Selection of the carrier gas to be used: ▪ **Air** ▪ **Nitrogen**

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

Oven / Gas Flow Unit – Properties (chapter 5.12.3.19, page 953)

Oven Unit – Manual control (chapter 5.12.3.19.1, page 954)

5.12.3.20 Pick&Place Module – Properties

After selecting the **Pick&Place Module** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for the **Beaker** in the **Specific data** subsection:

Beaker	
Beaker diameter	Diameter of a sample beaker in the beaker holder. Depending on the beaker size used, the following settings are recommended: ▪ 75 mL: **35.5 mm** ▪ 120 mL: **47.3 mm** ▪ 150 mL: **62.0 mm** ▪ 200 mL: **70.0 mm** ▪ 250 mL: **64.7 mm**
Beaker height	Height of the sample beakers in the beaker holder. The following settings are recommended for the used beaker sizes: ▪ 75 mL, 120 mL, 250 mL: **113.0 mm** ▪ 150 mL: **96.0 mm** ▪ 200 mL: **100.0 mm**

Modified data of the functional unit cannot be saved for as long as it is being used by a method in the process sequence.

5.12.3.20.1 Pick&Place Module – Manual control

If a functional unit of the **Pick&Place Module** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit appear in the **Manual control** window.

Status display

The current status of the Pick&Place module is visible on the icon display. Additionally, the current lift height is displayed in the status window.

Initializing

	Click this icon to initialize the Pick&Place module. During initialization, the status symbol of the Pick&Place module flashes **orange**. The lift of the Pick&Place module is moved right to the top (lift height 0 mm) and the slide is moved to the work position (rear). As soon as the initialization is complete, the status symbol lights up **green**. The status display on the instrument shows the alternating status of the Pick&Place module's status symbol at the same time.

If the Pick&Place module has already been initialized, the icon is grayed out.

Moving the lift

Lift height	Target height to which the lift is moved. A lift height of 0 mm corresponds to the home position at the top end stop of the lift.
	Click this icon to move the lift to the entered target height.
	Click this icon to cancel the process.
Speed	Speed at which the lift moves.

Move slide

Move slide	Move the slide of the Pick&Place module to the desired position.
	Click this icon to move the slide into the exchange position (front).
	Click this icon to move the slide into the work position (rear).

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

5.12.3.21 OMNIS Rod Stirrer – Properties

After selecting the **OMNIS Rod Stirrer** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for the **Operation of keys** of the rod stirrer in the **Specific data** subsection:

Operation of keys	Settings for the manual operation of keys of the rod stirrer.
Operation by	Selection of how the rod stirrer is operated manually: ▪ **No keys** The rod stirrer is operated solely using the software. ▪ **Keys on other stirrer** The rod stirrer is operated using the hardware buttons of the selected magnetic stirrer.
Other stirrer	Selection of the other magnetic stirrer with the hardware buttons of which the rod stirrer is to be operated.

For the control of a rod stirrer via the hardware buttons of a magnetic stirrer, only magnetic stirrers that are connected to the same OMNIS Titrator (or to the titration module or dosing module connected to this titrator) can be selected.

Please note that no modified data of the functional unit can be saved for as long as it is being used by a method in the process sequence.

See also

OMNIS Rod Stirrer – Manual control (chapter 5.12.3.21.1, page 958)

STIR – Properties (chapter 5.11.8.56, page 754)

5.12.3.21.1 OMNIS Rod Stirrer – Manual control

If a functional unit of the **OMNIS Rod Stirrer** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit appear in the **Manual control** window.

Status display

The current status of the stirrer is visible in the icon display. Additionally, the following information is displayed in the status window:

- Stirring rate
- Rotation direction

Switching on and off

	The stirrer is switched off. Click the switch to turn on the stirrer.
	The stirrer is switched on and runs until it is switched off again. Click the switch to turn the stirrer off.

Stirring rate

Stirring rate	Stirring rate (stirring level) and rotation direction of the stirrer. The following values can be entered: ▪ **+1** to **+15**: Stirring levels if the rotation direction of the solution is counterclockwise. ▪ **–1** to **–15**: Stirring levels if the rotation direction of the solution is clockwise.
	Increase stirring rate.
	Reduce stirring rate.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

5.12.3.22 801 Stirrer – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page*

865). The following functions and information are available for functional units of the **801 Stirrer** type in the **Specific data** subsection:

Specific data

Connector	
MSB connector	Number of the MSB connector on the Metrohm USB device that the functional unit is connected to.

See also

STIR – Properties (chapter 5.11.8.56, page 754)

5.12.3.23 Magnetic Stirrer – Properties

After selecting the **Magnetic Stirrer** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for the **Operation of keys** of the magnetic stirrer in the **Specific data** subsection:

Operation of keys	Settings for the manual operation of keys of the magnetic stirrer.
Operation by	Selection of how the magnetic stirrer is operated manually: ▪ **Keys on stirrer** The magnetic stirrer is operated using the hardware buttons on the functional unit. ▪ **No keys** The magnetic stirrer is operated solely using the software. The hardware buttons on the functional unit are not active. ▪ **Keys on other stirrer** The magnetic stirrer is operated using the hardware buttons of another magnetic stirrer.
Other stirrer	Selection of the other magnetic stirrer that is to be used for key operation.

Please note that no modified data of the functional unit can be saved for as long as it is being used by a method in the process sequence.

See also

801 Stirrer – Manual control (chapter 5.12.3.23.1, page 961)

Magnetic Stirrer – Manual control (chapter 5.12.3.23.2, page 962)

STIR – Properties (chapter 5.11.8.56, page 754)

5.12.3.23.1 801 Stirrer – Manual control

If a functional unit of the **801 Stirrer** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit appear in the **Manual control** window.

Status display

The current status of the stirrer is visible in the icon display. Additionally, the following information is displayed in the status window when the stirrer is switched on:

- Stirring rate
- Rotation direction

Switching on and off

	The stirrer is switched off. Click the switch to turn on the stirrer.
	The stirrer is switched on and runs until it is switched off again. Click the switch to turn the stirrer off.

Stirring rate

Stirring rate	Stirring rate (stirring level) and rotation direction of the stirrer. The following values can be entered: ▪ **+1** to **+15**: Stirring levels if the rotation direction of the solution is counterclockwise. ▪ **–1** to **–15**: Stirring levels if the rotation direction of the solution is clockwise.
	Increase stirring rate.
	Reduce stirring rate.

See also

801 Stirrer – Properties (chapter 5.12.3.22, page 959)

Magnetic Stirrer – Properties (chapter 5.12.3.23, page 960)

5.12.3.23.2 Magnetic Stirrer – Manual control

If a functional unit of the **Magnetic Stirrer** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit appear in the **Manual control** window.

Status display

The current status of the stirrer is visible in the icon display. Additionally, the following information is displayed in the status window:

- Stirring rate
- Rotation direction

Switching on and off

	The stirrer is switched off. Click the switch to turn on the stirrer.
	The stirrer is switched on and runs until it is switched off again. Click the switch to turn the stirrer off.

Stirring rate

Stirring rate	Stirring rate (stirring level) and rotation direction of the stirrer. The following values can be entered: ▪ **+1** to **+15**: Stirring levels if the rotation direction of the solution is counterclockwise. ▪ **–1** to **–15**: Stirring levels if the rotation direction of the solution is clockwise.
	Increase stirring rate.
	Reduce stirring rate.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

5.12.3.24 OMNIS Solvent Module – Manual control

If a **OMNIS Solvent Module** type functional unit is selected in the **Instruments** subsection, then the possible functions and parameters for the solvent module appear in the **Manual control** window.

Status display

The current status of the solvent module is visible in the icon display. Additionally, the following information is displayed in the status window:

- Current function (**Aspirate** or **Add**).
- Current status (**Pressure build-up**, **Pumping** or **Pressure release**).
- **Last Pumping duration**

Pump

These functions can be used in the following situations:

- Aspirate titrated solution from the titration cell.
- Pump new reagent into the titration cell.

	Click on this icon and continue to press down on it to start the **Aspirate** function.
	Click on this icon and continue to press down on it to start the **Add** function.

See also

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.3.25 804 Ti Stand – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **804 Ti Stand** type in the **Specific data** subsection:

Specific data

Connector	
MSB connector	Number of the MSB connector on the Metrohm USB device that the functional unit is connected to.

See also

STIR – Properties (chapter 5.11.8.56, page 754)

5.12.3.26 803 Ti Stand – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **803 Ti Stand** type in the **Specific data** subsection:

Specific data

Connector	
MSB connector	Number of the MSB connector on the Metrohm USB device that the functional unit is connected to.

See also

STIR – Properties (chapter 5.11.8.56, page 754)

5.12.3.26.1 804 Ti Stand – Manual control

If a **804 Ti Stand** type functional unit is selected in the **Instruments** subsection, then the possible functions and settings for the **802 Stirrer** connected to the titration stand appear in the **Manual control** window.

Status display

The current status of the stirrer is visible in the icon display. Additionally, the following information is displayed in the status window when the stirrer is switched on:

- Stirring rate
- Rotation direction

Switching on and off

	The stirrer is switched off. Click the switch to turn on the stirrer.
	The stirrer is switched on and runs until it is switched off again. Click the switch to turn the stirrer off.

Stirring rate

Stirring rate	Stirring rate (stirring level) and rotation direction of the stirrer. The following values can be entered: ▪ **+1** to **+15**: Stirring levels if the rotation direction of the solution is counterclockwise. ▪ **–1** to **–15**: Stirring levels if the rotation direction of the solution is clockwise.
	Increase stirring rate.
	Reduce stirring rate.

See also

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.3.26.2 803 Ti Stand – Manual control

If a **803 Ti Stand** type functional unit is selected in the **Instruments** subsection, then the possible functions and settings for the installed stirrer appear in the **Manual control** window.

Status display

The current status of the stirrer is visible in the icon display. Additionally, the following information is displayed in the status window when the stirrer is switched on:

- Stirring rate
- Rotation direction

Switching on and off

	The stirrer is switched off. Click the switch to turn on the stirrer.

	The stirrer is switched on and runs until it is switched off again. Click the switch to turn the stirrer off.

Stirring rate

Stirring rate	Stirring rate (stirring level) and rotation direction of the stirrer. The following values can be entered: ▪ **+1** to **+15**: Stirring levels if the rotation direction of the solution is counterclockwise. ▪ **–1** to **–15**: Stirring levels if the rotation direction of the solution is clockwise.
	Increase stirring rate.
	Reduce stirring rate.

See also

803 Ti Stand – Properties (chapter 5.12.3.26, page 964)

804 Ti Stand – Properties (chapter 5.12.3.25, page 963)

5.12.3.27 Pump module – Manual control

If a functional unit of the **Pump Module** type is selected in the instrument overview, the possible functions and parameters for the functional unit appear in the **Manual control** window.

Status display

The current status of the pump module is visible in the icon display.

Switching on and off

The pumps 1 - 4 on the selected pump module can be switched on and off manually.

	The pump is switched off. Click the switch to turn the pump on.

The pump is switched on and runs until it is switched back off.

Click the switch to turn the pump off.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

5.12.3.28 Membrane Pump (Aspirate) – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **Membrane Pump (Aspirate)** type in the **Specific data** subsection:

Specific data

Position	
Tower	Display the tower in which the membrane pump is installed.

See also

Instruments – Properties (chapter 5.12.2.5, page 865)

Membrane Pump (Aspirate) – Manual control (chapter 5.12.3.28.2, page 968)

Membrane Pump (Rinse) – Manual control (chapter 5.12.3.28.1, page 967)

PUMP – Properties (chapter 5.11.8.52, page 749)

5.12.3.28.1 Membrane Pump (Rinse) – Manual control

If a functional unit of the **Membrane Pump (Rinse)** type is selected in the overview of the instrument, the possible functions for the functional unit appear in the **Manual control** window.

Status display

The current status of the pump is visible in the icon display.

Switching on and off

	The pump is switched off. Click the switch to turn the pump on.
	The pump is switched on and runs until it is switched back off. Click the switch to turn the pump off.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

Instruments – Properties (chapter 5.12.2.5, page 865)

Membrane Pump (Aspirate) – Properties (chapter 5.12.3.28, page 967)

5.12.3.28.2 Membrane Pump (Aspirate) – Manual control

If a functional unit of the **Membrane Pump (Aspirate)** type is selected in the overview of the instrument, the possible functions for the functional unit appear in the **Manual control** window.

Status display

The current status of the pump is visible in the icon display.

Switching on and off

	The pump is switched off. Click the switch to turn the pump on.
	The pump is switched on and runs until it is switched back off. Click the switch to turn the pump off.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

Instruments – Properties (chapter 5.12.2.5, page 865)

Membrane Pump (Aspirate) – Properties (chapter 5.12.3.28, page 967)

5.12.3.29 Remote Box MSB – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page*

865). The following functions and information are available for functional units of the **Remote Box MSB** type in the **Specific data** subsection:

Specific data

Emergency stop	
Output signal	Output signal that is sent to the connected instrument via the Remote Box MSB if the emergency stop function is activated. A pre-defined output signal to stop pumps 1 and 2 of the **843 Pump Station** can be selected or a bit pattern for the output signal can be entered to control other instruments. The following pre-defined output signal to control the **843 Pump Station** is available: ▪ Instruments **843 - Pump 1 and Pump 2 off**: Stop of pump 1 and pump 2. Bit pattern for the output signal: ***00********* For controlling other instruments, a user-defined bit pattern can be entered manually under **Enter bit pattern**. If **Enter bit pattern** is selected, the following specific parameter appears: ▪ **Bit pattern**
Bit pattern	Entry of a user-defined bit pattern for the output signal. The bit pattern must contain 14 characters in total. The following characters may be used: ▪ **1** = Output line active ▪ **0** = Output line inactive ▪ ***** = Any status of the output line ▪ **p** = Set a pulse with a pulse duration of 200 ms
Connector	
MSB connector	Number of the MSB connector on the MSB device that the functional unit is connected to.

See also

REMOTE IN – Properties (chapter 5.11.8.74, page 790)

REMOTE OUT – Properties (chapter 5.11.8.75, page 792)

5.12.3.30 Tower – Properties

After selecting the **Tower** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **Tower** type in the **Specific data** subsection:

Specific data

Tower	
Maximum lift height	Enter the maximum height (in mm) to which the lift can be moved. A lift height of **0 mm** corresponds thereby to the home position at the top end stop of the lift.
Axial distance	Enter the distance between the axis of rotation of the sample rack and the center of the titration head or the swing axis of the robotic arm. Depending on the instrument version, the following default values apply for the axial distance: ▪ **814 USB Sample Processor** and **855 Robotic Titrosampler "Light"**: 166.0 mm ▪ **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler "Basic"**: 196.0 mm ***Note***: The **Axial distance** can only be adjusted for instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**.

Initial position	
Move to initial position after initialization	If this check box is enabled, an initial position can be defined. The lift and sample rack move to this position after the sample changer has been reserved or initialized or after the connection to the instrument has been re-established. If the initial position is disabled, then the sample rack is rotated to the starting position and the lift is moved to home position.

Initial position	
Movement target	Select the type of position that is to be approached: ▪ **Enter position on rack**: The movement target to be approached is an absolute position on the sample rack. ▪ **Special position**: The movement target to be approached is a special position that has been defined in the properties of the sample rack in **Positions on the rack**. ▪ **External position**: The movement target to be approached is an external position that has been defined in the properties of the **786 Swing Head**.
Target position or **Index**	Enter the target position or index number of the required special position or external position.
Target height	Select a defined height to which the lift is to be moved: ▪ **Work height**: Height that was defined for positions on the rack in the properties of the sample rack and for external positions in the properties of the 786 Swing Head as work height. ▪ **Special height**: Height that was defined in the properties of the sample rack as special height. ▪ **Rinse height**: Height that was defined for positions on the rack in the properties of the sample rack and for external positions in the properties of the 786 Swing Head as rinse height. ▪ **Enter height**: Entry of an absolute height to which the lift is to be moved. If **Enter height** is selected, the following specific parameter appears: – **Lift height**
Target height	Enter the absolute height to which the lift is to be moved. A lift height of **0 mm** corresponds thereby to the home position at the top end stop of the lift.

Parameters with different input ranges

Depending on the instrument used, different input ranges apply for the following parameters:

- **Maximum lift height**
  - **814 USB Sample Processor**:
    Minimum value: 0 mm
    Maximum value: 235 mm
  - **815 Robotic USB Sample Processor XL**:
    Minimum value: 0 mm
    Maximum value: 235 mm
  - **855 Robotic Titrosampler**:
    Minimum value: 0 mm
    Maximum value: 235 mm
  - **874 Oven Sample Processor**:
    Minimum value: 0 mm
    Maximum value: 155 mm

For the **874 Oven Sample Processor**, the maximum lift height is 110 mm for standard applications. Values above this may be used only for special applications.

See also

Defining the lift height (chapter 5.12.3.30.3, page 978)

External Pump Socket – Properties (chapter 5.12.3.30.5, page 984)

Membrane Pump (Aspirate) – Properties (chapter 5.12.3.28, page 967)

Reserving and releasing instruments (chapter 5.12.2.4, page 861)

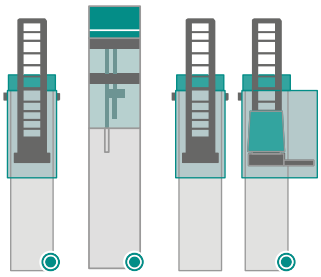
Tower Stirrer Socket – Properties (chapter 5.12.3.30.6, page 985)

Tower – Manual control (chapter 5.12.3.30.1, page 972)

5.12.3.30.1 Tower – Manual control

If a functional unit of the **Tower** type is selected in the **Instruments** subsection, then the possible functions, parameters and information for the functional unit appear in the **Manual control** window. Depending on the product type or instrument version, different functions and parameters are displayed.

Status display



The current status of the tower is visible in the icon display. Additionally, the following information is displayed in the status window:

- Lift height
- Position
- Angle

Initializing

	Click on this icon to initialize the tower. During the initialization, the status symbol of the tower flashes **orange**. As soon as the initialization of the tower is complete, the status symbol lights up **green**.

Selecting the tower

Click on the **[Tower 2]** or **[Tower 1]** button to select the tower that is to be operated manually.

Rotating the sample rack

Position on the rack	Select the position on the sample rack that is approached: ▪ **Special position**: Position that is defined in the properties of the sample rack as valid special position. If **Special position** is selected, the following specific parameter appears: – **Index** ▪ **Enter position**: Absolute position on the sample rack. If **Enter position** is selected, the following specific parameter appears: – **Target position**
Index	Enter the number of the special position (**1–16**). Special positions can be defined under **Equipment ▶ Sample racks ▶ Properties ▶ Positions on the rack** *(see "Defining a special position", chapter 5.12.3.30.4, page 982)*.
Target position	Enter the position on the sample rack. The position numbers are marked on the sample rack. The number of positions depends on the respective sample rack.
	Click on this icon to rotate the rack to the specified position on the sample rack.
	Click this icon to cancel the process.

Swinging the robotic arm

External position	Enter the index of the external position to which the robotic arm will swing.
	Click on this icon to swing the robotic arm to the entered external position.
	Click this icon to cancel the process.
Swing mode	Select the mode with which the robotic arm is to swing: ▪ **Relative angle**: Relative angle by which the robotic arm is swiveled from the current position. ▪ **Absolute angle**: Absolute angle to which the robotic arm is swiveled.
Angle	Depending on your selection, enter the relative angle by which the robotic arm is swiveled from the current position or enter the absolute angle to which the robotic arm is swiveled.
	Click on this icon to swing the robotic arm by or to the entered angle.
	Click this icon to cancel the process.
Swing rate	Rate at which the robotic arm is swiveled.

Moving the lift

Target height	Select a defined height to which the lift is moved: ▪ **Work height**: Height that is defined for positions on the rack in the properties of the sample rack and for external positions in the properties of the 786 Swing Head as work height. A separate work height can be defined for each special position and each external position. ▪ **Rinse height**: Height that is defined for positions on the rack in the properties of the sample rack and for external positions in the properties of the 786 Swing Head as rinse height. ▪ **Change height**: Height that is defined for positions on the rack in the properties of the sample rack as change height. ▪ **Special height**: Height that is defined for positions on the rack in the properties of the sample rack as special height. ▪ **Enter height**: Entry of an absolute height to which the lift is moved. If **Enter height** is selected, the following specific parameter appears: – **Lift height** ***Note***: If substitute values are selected, the lift uses the specific lift height that is defined for the position in which the lift is when the command is executed. Further information on defining lift heights: *(see "Defining the lift height", chapter 5.12.3.30.3, page 978)*.
Lift height	Enter the height (in mm) to which the lift is moved. A lift height of 0 mm corresponds thereby to the home position at the top end stop of the lift.
	Click this icon to move the lift to the selected or entered lift height.
	Click this icon to cancel the process.
Lift rate	Speed at which the lift is moved.

Park lift and sample rack (only 874 Oven Sample Processor)

	Click on this icon to move the lift and the sample rack into park position during ongoing operation. This ensures safe access to the working area (e.g. to remove the sample rack). The lift moves automatically into park position as soon as the operating procedure allows for it. Running methods are not interrupted. The parking procedure can be interrupted at any time. A message indicates that the park position has been reached and the access is safe. Initialize the lift after manipulation is complete (e.g. after replacing sample vessels) so that any waiting samples can be processed further.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

Tower – Properties (chapter 5.12.3.30, page 969)

5.12.3.30.2 786 Swing Head – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window. The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **786 Swing Head** type in the **Specific data** subsection:

Robotic arm configuration	
Swing direction	Select the swing direction of the robotic arm. **Note**: For the 2-tower version, the swing direction of the robotic arm must be **Negative** (-) at tower 1 and **Positive** (+) at tower 2.
Robotic arm offset	Enter the swing angle offset for a specific robotic arm model.
Maximum swing range	Enter the maximum usable swing range for a specific robotic arm model. **Note**: The maximum swing range depends on the construction of the robotic arm model and is defined by the maximum approachable angle.

Robotic arm configuration	
Swing radius	Enter the swing radius of the robotic arm. **Note**: The swing radius depends on the length of the robotic arm (from the axis of rotation to the center of the robotic arm tip) and, together with the axial distance, is the most important parameter for precisely approaching a rack position.
Rotation angle offset	Offset from the center of the tower to the center of the robotic arm, which corresponds to the default value when assembling the robotic arm without lateral offset. **Note**: If a robotic arm is mounted on the tower with a lateral offset, this value can be determined with a rack adjustment by the regional Metrohm service representative.

The values for the parameters of the robotic arm configuration must be entered according to the specifications in the product manual of the **786 Swing Head** (except for **Rotation angle offset**). The value for the **Maximum swing range** parameter can also be reduced if necessary.

External positions	
Swing height	Enter the height (in mm) that the lift is moved to for swinging the robotic arm to an external position or from an external position. If the lift is at a lower lift height than the swing height before the swing movement of the robotic arm, then the lift is automatically moved to the swing height. If the lift is at a higher lift height than the swing height, the swing movement is carried out at the current lift height. **Note**: If the swing height is lower than the change height, then the swing movement of the robotic arm takes place at the change height for safety reasons.

External positions	
Rinse height	Enter the height (in mm) that the lift is moved to in all external positions, for instance for cleaning electrodes, stirrers and buret tips. **Note**: This Rinse height only applies for external positions. The rinse heights for positions on the rack can be defined in the properties of the sample racks *(see "Defining the lift height", chapter 5.12.3.30.3, page 978)*.

External position 1–4	
Angle	Enter the angle to which the robotic arm is swiveled for moving to the external position.
Work height	Enter the work height (in mm) that the lift is moved to at the external position. This lift position can be used, for example, for pipetting samples. **Note**: A separate work height can be defined for each external position. The work heights for positions on the rack can be defined in the properties of the sample racks *(see "Defining the lift height", chapter 5.12.3.30.3, page 978)*.

External positions are positions next to the sample rack, e.g. an external rinsing station.

See also

Defining the lift height (chapter 5.12.3.30.3, page 978)

Functional unit – Directory (chapter 5.12.3.1, page 894)

Tower – Manual control (chapter 5.12.3.30.1, page 972)

5.12.3.30.3 Defining the lift height

Lift heights can be defined for the positions on the sample rack and for external positions of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**. The lift heights defined according to these instructions can be used as substitute values for the target height in the **LIFT** command and in the manual control.

Lift heights for positions on the rack

Lift heights for external positions

Lift heights for positions on the rack

The following lift heights can be defined for each sample rack and each tower:

- **Work height**
- **Rinse height**
- **Change height**
- **Special height**

Prerequisite:

- A sample rack is in place and has been detected. The lift heights are defined for each sample rack separately.
- The user has the **Operate instruments manually** and **Manage sample racks** rights.

1 Opening the manual control

- Select the **Tower** functional unit in **Equipment** ▶ **Instruments**.

  Click on to open the **Manual control** window.

2 Moving to the lift height

- If the 2-tower version of a sample changer is used, select the required tower.
- Move to the required lift height by entering the **Lift height** (in mm) in the input field. By manually approaching and reading out the displayed lift height, the values for the following lift heights can be determined:
  - **Work height**: The electrodes, stirrers and buret tips should be positioned at this lift position for analysis. If the vessel sensor of the robotic arm is activated, the work height must be defined in such a way that there is contact between the vessel sensor and the sample vessel.
  - **Rinse height**: The electrodes, stirrers and buret tips should be positioned at this lift position for cleaning and the aspiration tip and the spray nozzles should be positioned as low as possible in the sample vessel.
  - **Change height**: The sample rack should rotate freely and the collision of electrodes, stirrers or buret tips with sample vessels should be prevented at this lift position.
  - **Special height**: This lift position can be used, for example, to immerse a pipetting tip.
- Make note of the value of the lift height.

3 Entering the lift height

- Select the sample rack under **Equipment** ▶ **Sample racks**.
- Click on to open the **Properties** window and select the **Positions on the rack** subsection.
- Expand the **Tower 1** or **Tower 2** parameter group in the **Positions on the rack** subsection.
- Enter the noted values for the lift heights in the respective input fields.

The **Positions on the rack** subsection is only available under **Equipment** ▶ **Sample racks** for instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**.

4 Saving the lift height

- Save the entry by clicking on .

The lift heights have been defined and can now be used for the positions on the selected sample rack.

A separate work height can be defined for each special position. The rinse height, the change height and the special height apply for all positions on the sample rack, this includes sample positions as well as special positions.

Lift heights for external positions

The following lift heights can be defined for each 786 Swing Head:

- **Swing height**
- **Rinse height**
- **Work height**

Prerequisite:

- A 786 Swing Head is mounted, connected and has been detected.
- The user has the **Operate instruments manually** and **Manage instruments** rights.

1 Opening the manual control

- Select the **Tower** functional unit in **Equipment** ▶ **Instruments**.

  Click on to open the **Manual control** window.

2 Moving to the lift height

- If the 2-tower version of a sample changer is used, select the required tower.
- Move to the required lift height by entering the **Lift height** (in mm) in the input field. By manually approaching and reading out the displayed lift height, the values for the following lift heights can be determined:
  - **Swing height**: The robotic arm should be able to swing freely between the external positions and the sample rack in this lift position.
  - **Rinse height**: The electrodes, stirrers and buret tips should be positioned at this lift position for cleaning.
  - **Work height**: This lift position can be used, for example, for pipetting samples.
- Make note of the value of the lift height.

3 Entering the lift height

- Select the **Tower** functional unit in **Equipment** ▶ **Instruments**.
- Click on to open the **Properties** window and select the **Specific data** subsection.
- In the **Specific data** subsection, expand the **External positions** and **External position 1–4** parameter groups in the section for the 786 Swing Head.
- Enter the noted values for the lift heights in the respective input fields.

4 Saving the lift height

- Save the entry by clicking on .

The lift heights have been defined and can now be used for external positions.

See also

Assigning the lift height (chapter 5.12.3.18.2, page 952)

Defining a special position (chapter 5.12.3.30.4, page 982)

LIFT – Properties (chapter 5.11.8.48, page 738)

Sample rack – Properties (chapter 5.12.8.2, page 1025)

Tower – Manual control (chapter 5.12.3.30.1, page 972)

5.12.3.30.4 Defining a special position

Special positions can be defined for sample racks of the **Sample Processor Rack** type of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**. The special positions defined according to these instructions are used for moving to special positions in the **MOVE TO RACK** command and in the manual control.

Prerequisite:

- A sample rack is in place and has been detected. The special positions are defined for each sample rack separately.
- The user has the **Manage sample racks** right.

1 Adding a special position

- Select the sample rack under **Equipment** ▶ **Sample racks**.
- Click on to open the **Properties** window and select the **Positions on the rack** subsection.
- Add a special position by clicking on .

A special position can be removed again by clicking .

2 Entering a position

- Enter the position on the rack that is to be defined as special position in the **Position** field.

Special positions should be defined preferably at high rack positions in order to be able to start sample series at the position 1. Positions on the rack that have been defined as special positions cannot be used as sample positions anymore in the subsample data.

0 can be defined as position in order to deactivate a special position temporarily and to prevent the special position from being deleted and thus the index to be reassigned and the defined lift heights to be lost. Special positions with position **0** cannot be used in the **MOVE TO RACK** command or in the manual control.

3 Activating the vessel sensor

- Click on ⌄ in the **Vessel sensor** field to select or deactivate the vessel sensor:
  - **Tower**: Activate the vessel sensor installed in the tower. Only positions on single-row sample racks can be checked.
  - **Robotic arm**: Activate the vessel sensor installed in the robotic arm. The work height must be defined in such a way that there is contact between the robotic arm and the sample vessel. The work height will be approached automatically after the **MOVE TO RACK** command.
  - **Off**: Deactivate vessel sensor.

If a position on the sample rack is approached with a **MOVE TO RACK** command or in the manual control, the vessel sensor checks if a vessel is present at the selected position.

The vessel sensor can be activated or deactivated for each special position regardless of the settings for the other positions on the rack.

This parameter is identical with the **Beaker sensor** parameter used in previous Metrohm applications. The designation **Vessel sensor** in the OMNIS Software corresponds to the designation **Beaker sensor** used in the product manual.

4 Defining the work height

- Expand the **Tower 1** or **Tower 2** parameter group in the subsection of the special position.
- Enter the required **Work height** (in mm) for the special position.

A separate work height can be defined for each special position. The rinse height, change height and special height are defined in **Equipment** ▶ **Sample racks** ▶ **Properties** ▶ **Positions on the rack** and apply for all positions on the rack *(see "Defining the lift height", chapter 5.12.3.30.3, page 978)*.

5 Saving the special position

- Save the special position by clicking on 🖬.

The special position is defined and can now be used in the **MOVE TO RACK** command and in the manual control.

Up to 16 special positions can be defined for each sample rack.

See also

Defining the lift height (chapter 5.12.3.30.3, page 978)

MOVE TO RACK – Properties (chapter 5.11.8.50, page 744)

Sample rack – Properties (chapter 5.12.8.2, page 1025)

5.12.3.30.5 External Pump Socket – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **External Pump Socket** type in the **Specific data** subsection:

Specific data

Position	
Tower	Display the tower in which the pump connector is installed.

The pump connected to the **External Pump Socket** is not recognized by the OMNIS Software and has no influence on the displayed product name or other properties of the functional unit.

See also

External Pump Socket – Manual control (chapter 5.12.3.30.5.1, page 984)

Functional unit – Directory (chapter 5.12.3.1, page 894)

Instruments – Properties (chapter 5.12.2.5, page 865)

PUMP – Properties (chapter 5.11.8.52, page 749)

5.12.3.30.5.1 External Pump Socket – Manual control

If a functional unit of the **External Pump Socket** type is selected in the overview of the instrument, the possible functions and parameters for the connected pump (772 Pump Unit, 823 Membrane Pump Unit or 843 Pump Station) appear in the **Manual control** window.

Status display

The current status of the pump is visible in the icon display.

Switching on and off

	The pump is switched off. Click the switch to turn the pump on.

The pump is switched on and runs until it is switched back off.

Click the switch to turn the pump off.

See also

External Pump Socket – Properties (chapter 5.12.3.30.5, page 984)

Functional unit – Directory (chapter 5.12.3.1, page 894)

Functional unit – Status (chapter 5.12.3.2, page 904)

Instruments – Properties (chapter 5.12.2.5, page 865)

5.12.3.30.6 Tower Stirrer Socket – Properties

Clicking on under **Equipment** ▶ **Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available for functional units of the **Tower Stirrer Socket** type in the **Specific data** subsection:

Specific data

Position	
Tower	Display the tower in which the stirrer connector is installed.

The stirrer connected to the **Tower Stirrer Socket** is not recognized by the OMNIS Software and has no influence on the displayed product name or other properties of the functional unit.

If an MSB stirrer is connected to the MSB connector 1 of a USB Sample Processor, then the stirrer connector of tower 1 cannot be used. If an MSB stirrer is connected to the MSB connector 2 of a USB Sample Processor in the 2-tower version, then the stirrer connector of tower 2 cannot be used.

See also

Instruments – Properties (chapter 5.12.2.5, page 865)

STIR – Properties (chapter 5.11.8.56, page 754)

Tower Stirrer Socket – Manual control (chapter 5.12.3.30.6.1, page 986)

5.12.3.30.6.1 Tower Stirrer Socket – Manual control

If a **Tower Stirrer Socket** type functional unit is selected in the **Instruments** subsection, then the possible functions and settings for the connected stirrer appear in the **Manual control** window.

Status display

The current status of the stirrer is visible in the icon display. Additionally, the following information is displayed in the status window when the stirrer is switched on:

- Rotation direction
- Stirring rate

Switching on and off

	The stirrer is switched off. Click the switch to turn on the stirrer.
	The stirrer is switched on and runs until it is switched off again. Click the switch to turn the stirrer off.

Stirring rate

Stirring rate	Stirring rate (stirring level) and rotation direction of the stirrer. The following values can be entered: ▪ **+1** to **+15**: Stirring levels if the rotation direction of the solution is counterclockwise. ▪ **–1** to **–15**: Stirring levels when the rotation direction of the solution is clockwise.
	Increase stirring rate.
	Reduce stirring rate.

See also

Functional unit – Status (chapter 5.12.3.2, page 904)

Instruments – Properties (chapter 5.12.2.5, page 865)

Tower Stirrer Socket – Properties (chapter 5.12.3.30.6, page 985)

5.12.4 Work system – Definition

A work system is a compilation of functional units of the instruments reserved by the user. To be able to analyze subsamples with an operating procedure, at least one work system must be assigned to each method contained in this operating procedure. Functional units from the work system which are required for executing the method are then defined in the commands contained in the method.

Overview list

The following information is displayed by default in the overview list of the work systems:

	The symbol is displayed if a functional unit of the work system is not available, has not yet been initialized, is faulty or has an incompatible firmware.
Name	Name of the work system that can be modified in the properties of the work system as needed.
Saved	Date of the last modification of the work system.

See also

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Creating a work system (chapter 5.12.4.4, page 989)

Equipment – Inventory (chapter 5.12.1, page 852)

Functional unit – Manual control (chapter 5.12.3.5, page 906)

Removing a work system from a method (chapter 5.12.4.6, page 992)

Work system – Properties (chapter 5.12.4.2, page 988)

5.12.4.1 Work systems – Subsection

The following functions are available in **Equipment** ▶ **Work systems**:

-

  Assemble work systems is used to assemble a work system for executing a method made up of functional units.

-

  Delete work system is used to delete the work system. If a method to which the work system is assigned is to be used in a determination, then a new work system must be assigned to it.

Overview list

The following information is displayed in the overview list:

	The symbol is displayed if a functional unit of the work system is not available, has not yet been initialized, is faulty or has an incompatible firmware.
Name	Name of the work system. The name can be adjusted after opening the work system.
Published	Status of the work system in the **OMNIS Client/Server system**. Additional information: *(see "Work system – Status", chapter 5.12.4.3, page 989)* **Note**: Applicable only in the **OMNIS Client/Server system**.
Saved	Time at which the method was last saved.

See also

Creating a work system (chapter 5.12.4.4, page 989)

5.12.4.2 Work system – Properties

Clicking on in **Equipment** ▶ **Work system** opens the **Properties** window. For the work system or the selected functional unit, the following functions are available in the **General** subsection:

General

Name	Name of work system or the functional unit (can be edited, max. 255 characters).
Object ID	Identification number of the work system.
Connected to instrument / module	Product name of the instrument which includes the functional unit or which it is connected to.

- It is not imperative for the names for work systems and functional units to be unique. The same name can thus be assigned several times for the same element. We recommend, however, that unique names be assigned wherever possible.
- The names that are entered for the individual functional units in the work system only apply in the respective work system. This means that the same functional unit can also have different names in different work systems.

See also

Creating a work system (chapter 5.12.4.4, page 989)

Work system – Definition (chapter 5.12.4, page 987)

5.12.4.3 Work system – Status

In the **OMNIS Client/Server system**, every work system that is on the OMNIS Server has a status. This is displayed under **Equipment** ▶ **Work systems** in the **Published** column.

Published	Meaning
	Published The work system is published.

If the work system is not published, then the **Published** column is empty.

See also

Determination – Definition (chapter 5.10.8, page 295)

Determination – Preparation and follow-up (chapter 5.10.8.10, page 313)

Preparing determination (chapter 5.10.8.9, page 310)

5.12.4.4 Creating a work system

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- An instrument has been reserved.

1 Setting up a work system

- In **Equipment** ▶ **Work systems**, click on .

A new tab opens with **New work system** as its title.

2 Naming a work system

- Click on to open the **Properties** window.
- Enter the desired name for the work system in the **Name** field in **Properties** ▶ **General**.

3 Inserting functional units

- Click on to open the **Inventory** window.

- Use drag and drop to insert the desired functional units into the work system. The sequence in which the functional units are added to the work system plays no role in this connection.

4 Removing functional units

- Remove the desired functional units from the work system once again by clicking ✕.

Functional units that are already assigned to one or more commands can also be deleted. The assignment of the functional unit to the commands is deleted automatically in such cases without a new method version being generated thereby.

5 Naming functional units

- Select the functional unit whose name is to be changed.
- Click on to open the **Properties** window.
- Enter the desired name for the functional unit in the **Name** field in **Properties** ▶ **General**.

6 Saving a work system

- Save the work system by clicking on .

One functional unit can be assigned to several work systems.

If the selected work system is being used for conditioning, the current measured values for the ongoing conditioning process are displayed in **Current status**.
Additional information on the conditioning: *(see "Karl Fischer titration – Principle", chapter 5.11.8.9, page 561), (see "Conditioning – Principle", chapter 5.11.8.10, page 567)*

See also

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Removing a work system from a method (chapter 5.12.4.6, page 992)

Reserving and releasing instruments (chapter 5.12.2.4, page 861)

5.12.4.5 Assigning a work system to a method

Assigning work systems to methods defines which functional units to use to execute the individual commands within methods.

Multiple work systems can be assigned to a method. This allows you to run commands of the same method with functional units of different work systems, depending on availability. This is particularly useful if the

same analyses are performed at multiple work stations of the sample robot.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

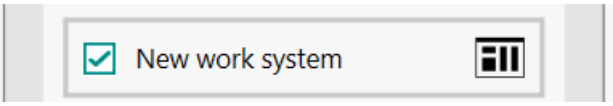
1 Opening a method

- Select the required method in **Processes** ▶ **Methods** and open it with a double-click.

A new tab opens with the selected method as its title.

2 Assigning a work system

- Click on to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.
- Enable the check box next to the work system that you would like to assign to the method.



3 Saving a method

- Save the method by clicking on .

The method is saved. At the same time, the method's new version number and the new version date are entered automatically in the **General** subsection of the **Properties** window.

If a work system contains more than one functional unit of the same type, then the desired functional unit will need to be assigned manually to the command.

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

Creating a work system (chapter 5.12.4.4, page 989)

Creating and editing a method (chapter 5.11.3.3, page 418)

Method – Properties (chapter 5.11.3.2, page 416)

Removing a work system from a method (chapter 5.12.4.6, page 992)

5.12.4.6 Removing a work system from a method

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Opening a method

- Double-click to open the required method in **Processes** ▶ **Methods**.

A new tab with the title of the selected method opens.

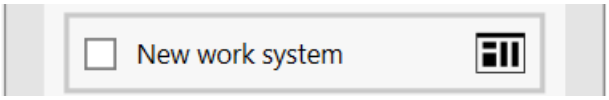
2 Opening Properties

- Click on to open the **Properties** window.
  or
- Double-click on

to open the **Properties** window.

3 Removing a work system

- In the **Properties** window, select the **Execute with** subsection.
- Disable the check box next to the work system that you want to remove from the method.



4 Saving a method

- Save the method by clicking on .

The method is saved. At the same time, the method's new version number and the new version date are entered automatically in the **General** subsection of the **Properties** window.

See also

Assigning a work system to a method (chapter 5.12.4.5, page 990)

Creating a work system (chapter 5.12.4.4, page 989)

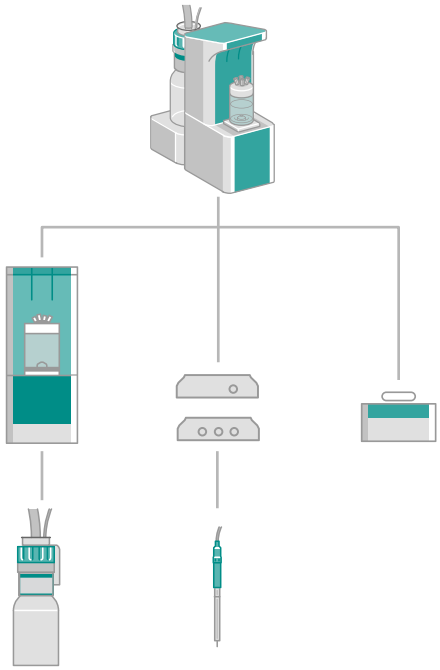
Method – Properties (chapter 5.11.3.2, page 416)

5.12.5 Additional component – Definition

An additional component is a flexible component (e.g. sensor, solution, or sample rack) of a functional unit which is used together with the associated functional unit to execute commands. Additional components are displayed in the overview of the instrument and can be managed in the **Equipment** work area. When a user reserves an instrument, all additional components of that instrument are available to that user, along with the respective functional unit.

Example: Titrator with two additional components

- OMNIS Liquid Adapter with connected solution with bottle cap multi-use
- Digital sensor



See also

Additional component – Directory (chapter 5.12.5.1, page 993)

Functional unit – Manual control (chapter 5.12.3.5, page 906)

Functional unit – Status (chapter 5.12.3.2, page 904)

5.12.5.1 Additional component – Directory

- *Additional components for OMNIS instruments*
- *Additional components for Metrohm USB instruments*

Additional components for OMNIS instruments

Analog sensors

Analog sensors of the other sensor, ion-selective electrode, metal electrode and pH electrode types can be connected to a **Measuring Module Analog** measuring module.

Analog sensors of the polarizable metal electrode and temperature sensor types can be connected to a **Measuring Module Analog** or a **Measuring Module Coulometry** measuring module.

Analog sensors of the conductivity measuring cell type can be connected to a **Measuring Module Conductivity** measuring module.

The data for an analog sensor must be recorded manually in the **Properties** window of the sensor in the 2 subsections **General** and **Specific data**.

Analog sensors can be added to the overview list of the sensors in **Equipment** ▶ **Sensors** ▶ **Inventory** ▶ **Analog sensors** using drag and drop.

dTrode

The digital sensor of the **dTrode** type can be connected to a measuring module of the **Measuring Module Digital** type. As soon as the sensor is connected, it is displayed automatically in the overview of the instrument and in the overview list of the sensors. The following sensor types are available: ion-selective electrode, metal electrode, pH electrode and Thermoprobe.

A measuring interface and a memory chip are installed in the sensor on which all sensor data is saved. The data extracted from the memory chip is displayed in the properties of the sensor.

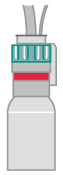
Conductivity standard

Conductivity standards are required for conductivity calibrations. The template for conductivity standards is stored in **Equipment** ▶ **Solutions** ▶ **Inventory**. Conductivity standards can be added to the overview list of the solutions and managed from there.

Solution with bottle cap multi-use

Bottle caps multi-use are designed for multiple use with different solutions. As soon as the solution with the bottle cap multi-use is connected to the **OMNIS Liquid Adapter**, it is displayed automatically in the overview of the instrument and included in the overview list of the solutions.

The bottle cap has a memory chip to which the solution data is saved. The solution data is read out from the attached Liquid Adapter, which transmits the data to the OMNIS Software. The properties of the solution can be edited and stored on the memory chip.



Solution with bottle cap single-use

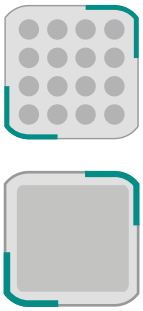
The bottle is delivered by the manufacturer with bottle cap single-use mounted. As soon as the solution with the bottle cap single-use is connected to the **OMNIS Liquid Adapter**, it is displayed automatically in the overview of the instrument and included in the overview list of the solutions.

The bottle cap contains a memory chip containing information (such as solution name, concentration, concentration unit, etc.) which is defined by the manufacturer and cannot be changed. Other properties of the solution (e.g. titer, titer unit) can be edited. The information on the memory chip is read out from the attached Liquid Adapter, which transmits the data to the OMNIS Software. The bottle cap single-use cannot be removed from the bottle without making the memory chip unusable.

OMNIS Liquid Adapter

The OMNIS Liquid Adapter is used to connect solutions with the bottle cap multi-use or solutions with the bottle cap single-use.

The OMNIS Liquid Adapter contains an RFID reader that extracts the information saved on the memory chip of the bottle cap and transfers it to the OMNIS Software.



OMNIS Sample Rack

The sample rack of the **OMNIS Sample Rack** type is used for holding sample vessels and is placed on the rack base of the **OMNIS Sample Robot**, **OMNIS Sample Robot NIR** or **OMNIS Sample Robot Oven**. A beep sound confirms that it has been recognized by the sample robot. The sample rack is displayed automatically in the overview of the instrument and in the overview list of the sample racks. The sample rack is available for various vessel sizes.

In the overview of the instrument, the sample rack with the corresponding number of positions for sample vessels on the rack is displayed. No positions on racks are displayed for customized sample racks.

The sample rack contains a memory chip on which the data of the sample rack is stored.

Additional components for Metrohm USB instruments

Analog sensors

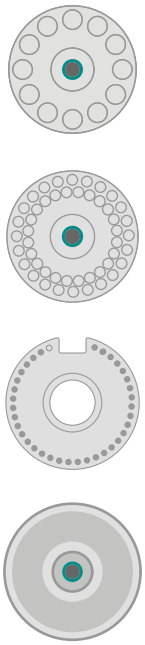
Analog sensors of the type other sensor, ion-selective electrode, metal electrode, pH electrode, polarizable metal electrode and temperature sensor can be connected to a measuring module **Measuring Interface Analog**. Analog sensors of the type polarizable metal electrode and temperature sensor can be connected to a **Interface Coulometry** measuring module. Analog sensors of the conductivity measuring cell type can be connected to a **Measuring Interface Conductivity** measuring module.

Note: The recording of the data and the addition to the overview list proceeds the same way as with the analog sensors for OMNIS instruments (*see above*).

iTrode

The intelligent sensor of the **iTrode** type can be connected to instruments of the **Titrando** type using a **Measuring Interface iConnect**. As soon as the **Measuring Interface iConnect** is connected with the sensor on the device, the sensor will be displayed automatically in the overview of the instrument and in the overview list of the sensors. The following sensor types are available: pH electrode and metal electrode.

This sensor has a built-in memory chip which is read out by the **Measuring Interface iConnect**. The data extracted from the memory chip is displayed in the properties of the sensor.



Sample Processor Rack

The single-row or multi-row sample rack of the **Sample Processor Rack** type is used for holding sample vessels and is placed on the turntable of the **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL**, **855 Robotic Titrosampler** or **874 Oven Sample Processor**. The sample rack is displayed automatically in the overview of the instrument and in the overview list of the sample racks as soon as the sample rack is placed on the turntable of the sample changer and this is initialized. The sample rack is available for various sample vessel sizes.

In the overview of the instrument, the sample rack with the corresponding number of positions for sample vessels on the rack is displayed. No positions on racks are displayed for customized sample racks.

The sample rack has a magnet code which is used to read the article number. The properties of the sample rack can be edited and stored on the local computer.

Solution IDU/IEU

Solutions which are connected to dosing drives of the type **800 Dosino** with connected **807 Dosing Unit**, **805 Dosimat** with connected **806 Exchange Unit** or **Internal Dosing Drive** with connected **806 Exchange Unit** are recognized by the OMNIS Software and displayed automatically in the overview of the instrument and in the overview list of the solutions.

The bottle has no memory chip. This solution data is saved on the memory chip of the **807 Dosing Unit** or the **806 Exchange Unit**. The properties of the solution can be modified and stored on the local computer.

See also

Sample rack – Definition (chapter 5.12.8, page 1023)

Sample rack – Status (chapter 5.12.8.3, page 1030)

Sensor – Definition (chapter 5.12.6, page 998)

Sensor – Status (chapter 5.12.6.3, page 1007)

Solution – Definition (chapter 5.12.7, page 1012)

Solution – Status (chapter 5.12.7.3, page 1019)

5.12.6 Sensor – Definition

A sensor is used for measuring physical or chemical properties. Digital, intelligent and analog sensors can be used in the OMNIS system.

The following sensor types are available:

- **Other sensor**: Sensor (not further specified) which delivers . potential (in mV) as measuring signal (e.g. optical sensor).
- **Ion-selective electrode**: Electrode for concentration measurements and potentiometric titrations of specific ions.
- **Conductivity measuring cell**: Measuring cell for measuring the conductivity of a solution.
- **Metal electrode**: Electrode for potentiometric measurements for redox titrations and precipitation titrations.
- **pH electrode**: Electrode for potentiometric pH measurements and acid-base titrations.
- **Polarizable metal electrode**: Electrode for voltametric or amperometric measurements for redox titrations with selectable polarization.
- **Temperature sensor**: Sensor for temperature measurement.

Additional information regarding the various product types: *(see "Additional component – Directory", chapter 5.12.5.1, page 993)*

See also

Enabling monitoring (chapter 5.7, page 193)

Equipment – Inventory (chapter 5.12.1, page 852)

Ion-selective electrode – Calibrating (chapter 5.12.6.5, page 1010)

Sensor – Status (chapter 5.12.6.3, page 1007)

pH electrode – Calibrating (chapter 5.12.6.4, page 1008)

5.12.6.1 Sensors – Subsection

The following functions are available in **Equipment** ▶ **Sensors**:

- **Define advance warning time** is used to define the advance warning time for the expiry date of the sensors.
- Use **Save** to save all changes.
- The view is reloaded with **Update view**. Unsaved entries are reset to the last saved version.
- Use **Remove sensors** to remove all selected spectra. If sensors of the **dTrode** or **iTrode** type are removed, then the data is retained on the memory chip. If sensors of the type **Analog Electrode** are removed, then the data saved in the OMNIS Software is deleted.

In addition, the following windows can be opened:

- The selection of all available sensors is displayed in the **Inventory** window.
- The properties of the selected element are displayed in **Properties**.

Overview list

The following information is displayed in the overview list:

	Status display for digital or intelligent sensors. ▪ **Green icon:** The sensor is connected to a **Measuring Module Digital** or a **Measuring Interface iConnect**. ▪ **Gray icon:** The sensor is not connected to either a **Measuring Module Digital** or a **Measuring Interface iConnect**.
Sensor type	Type of sensor, e.g. metal electrode, pH electrode, etc.
Product type	Type of signal transmission of the sensor. Digital sensors are designated with **dTrode**, intelligent sensors with **iTrode** and analog sensors with **Analog Electrode**.
Name	Name of the sensor. The sensor name corresponds to the sensor type in the default settings. The name can be adapted in the properties of the sensor.
Connected to	Measuring input to which the sensor is connected.
Calibration date	Date on which the calibration was carried out.
Calibration expiry date	Calibration expiry date. The monitoring status of the calibration is displayed with an icon that varies in accordance with status.
Sensor expiry date	Expiry date of the sensor. The monitoring status of the sensor is displayed with an icon that differs based on status.

New digital and intelligent sensors are detected automatically by the OMNIS Software and displayed in the overview list as soon as they have been connected for the first time. Analog sensors can be added to the overview list from the inventory using drag and drop. Sensors can be removed from the overview list if they are no longer being used in determinations. In addition, digital sensors may also no longer be connected to a **Measuring Module Digital** or a **Measuring Interface iConnect**.

See also

Sensor – Properties (chapter 5.12.6.2, page 1001)

5.12.6.2 Sensor – Properties

Clicking on under **Equipment** ▶ **Sensors** opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 2 subsections **General** and **Specific data**.

- To change the properties of a digital sensor or of an intelligent sensor, the sensor must be connected to the measuring module or measuring interface of a reserved instrument.
- Modified data of a digital or intelligent sensor cannot be saved as long as the measuring module or measuring interface is being used in a running determination.

General

The **Product information** and **Production data** parameter groups and are displayed for all digital, intelligent and analog sensors.

Product information	
Product name	Enter the name of the sensor. With digital and intelligent sensors, the product name is stored on the internal memory chip. With analog sensors, the product name is stored on the local computer.
Product type	Display the English designation of the sensor.
Sensor type	Display the sensor type.
Production data	
Article number	Display the number that unambiguously identifies the sensor. For analog sensors, the article number can be entered.
Serial number	Display the serial number of the sensor. For analog sensors, the serial number can be entered.

Specific data

Sensor data

The **Sensor data** parameter group is displayed for all digital, intelligent and analog sensors.

Start-up	Display the date of the start-up. With analog sensors, the date of start-up is set when the sensor is added to the sensor list. For a digital or intelligent sensor, the date of start-up is set as soon as it is used for the first time for a measurement or as soon as an editable field in its properties is changed.
Working life	Enter the working life of the sensor in days. Alternatively, the date selection can be used to define the working life.
Expiry date	Display the expiry date of the sensor. The expiry date is calculated using the date of initial start-up and the working life entered.
Enable monitoring	Enable sensor monitoring. If sensor monitoring is activated, then the monitoring status is indicated with a colored status icon in the **Sensor expiry date** table column in the sensor list. *(see "Sensor – Status", chapter 5.12.6.3, page 1007)*
Comment	Enter a comment (optional). Comment length: max. 250 characters.
Ion (only ion-selective electrode)	Select the ion for which the concentration is to be determined with the electrode.
Ion charge (only ion-selective electrode)	Display the charge of the selected ion. The ion charge is automatically adapted to the selected ion. If **Other ion** is selected For **Ion**, then the value of the ion charge can be entered manually in the range between 5+ and 5-.

Temperature sensor

The **Temperature sensor** parameter group is displayed for the following sensors:

- All digital and intelligent sensors of the pH electrode, ion-selective electrode and Thermoprobe types.
- All analog sensors of the pH electrode, ion-selective electrode and temperature sensor types.
- Conductivity measuring cells.

Type of temperature sensor	Display the type of the temperature sensor.
R (25 °C)	With temperature sensors of the NTC-B type, the nominal resistance must be specified at 25 °C (R(25 °C)).
B value	The thermistor constant (B value) must be specified for temperature sensors of the NTC-B type. The thermistor constant is a material constant.
Temperature correction (only digital and analog pH electrodes, digital and analog ion-selective electrodes, analog temperature sensors and conductivity measuring cells)	Enter the temperature offset by which the measured temperature is corrected. The temperature correction is used only for sensors that are connected to the measuring module of an OMNIS instrument. For some **conductivity measuring cells** with a cable length of 2 m, a temperature correction of –0.2 °C must be entered.

Article number	Cable length / m	Temperature correction / °C
6.0920.100	2.00	0
6.0920.130	2.00	0
6.00921.040	0.65	0
6.00922.040	2.00	–0.2
6.00923.080	0.65	0
6.00924.080	2.00	–0.2
6.00925.100	0.65	0
6.00929.140	0.65	0
6.00930.140	2.00	–0.2

Reference electrode

The **Reference electrode** parameter group is displayed for all digital sensors of the dTrode type (except Thermoprobe) as well as for analog ion-selective electrodes and analog metal electrodes.

Article number (only analog metal electrode and analog ion-selective electrode)	Display or enter the number that unambiguously identifies the reference electrode.
Serial number (only analog metal electrode and analog ion-selective electrode)	Display or enter the serial number of the reference electrode.
Reference electrolyte type	Select the reference electrolyte type (aqueous, nonaqueous, gel).
Reference electrolyte	Enter the electrolyte that is used in the reference electrode.
Bridge electrolyte type	Select the bridge electrolyte type (aqueous, nonaqueous, gel, not available).
Bridge electrolyte	Enter the electrolyte that is used between the reference electrode and the measuring electrode.

Calibration data

The **Calibration data** parameter group is displayed for all ion-selective electrodes, conductivity measuring cells, pH electrodes and Thermoprobes.

Slope (only pH electrode and ion-selective electrode)	Determine the slope of the sensor, either by performing a calibration or by entering it manually.
pH(0) (only pH electrode)	Determine the pH value for a potential of 0 mV, either by performing a calibration or by entering it manually.

E(0) (only ion-selective electrode)	Determine the electrode zero point, either by performing a calibration or by entering it manually. The electrode zero point corresponds to the y-intercept of the calibration curve (potential at log c = 0).
c(blank) (only ion-selective electrode)	Enter the blank value concentration c(Blind). The concentration of a blank is subtracted from the analysis result.
Unit (only ion-selective electrode)	Select or enter the unit for the ion concentration. It is possible thereby to choose between substance concentration, mass concentration and percentage. In addition, the default value can be selected or an individual value can be entered.
Variance (only pH electrode and ion-selective electrode)	Display the variance as a measure of dispersion. The measure of dispersion designates the distribution of values around the mean value. The variance has no unit.
Coefficient of determination (only pH electrode and ion-selective electrode)	Display the coefficient of determination R^2. The coefficient of determination is a statistical quantity or key figure for assessing how well measured values fit into a regression model. The coefficient of determination has no unit.
Cell constant (only conductivity measuring cell)	Determine the resistivity of the conductivity measuring cell used, either by performing a calibration or by entering it manually.
Calibration temperature	Enter the temperature of the 1st calibration buffer or the 1st calibration standard which was measured with a temperature sensor or entered manually during the calibration.
Temperature sensor	Display the temperature sensor (Pt1000 or NTC) with which the temperature was measured. **Manual** means that the temperature was entered manually.
User ID	Display the ID of the user who carried out the calibration or manually entered the calibration data.
Calibration date	Display the date on which the calibration was carried out or the calibration data was manually entered.

Validity period	Enter the validity period of the sensor calibration in hours.
Expiry date	Display the calibration expiry date. The expiry date is calculated using the calibration date and the validity period entered.
Enable monitoring	Activate the monitoring of calibration validity. If sensor monitoring is activated, then the monitoring status is indicated with a colored status icon in the **Calibration expiry date** table column in the sensor list. *(see "Sensor – Status", chapter 5.12.6.3, page 1007)*
Subsample ID	Display the object ID of the last subsample with which the calibration was carried out.
Comment on the calibration	Enter a comment (optional). Comment length: max. 250 characters.
Temperature T1 (only Thermoprobe)	First temperature at which the NTC thermistor was calibrated. The value was measured during calibration by the manufacturer and cannot be changed.
Resistance at T1 (only Thermoprobe)	Resistance of the NTC thermistor that was measured at the 1st temperature during calibration. The value was measured during calibration by the manufacturer and cannot be changed.
Temperature T2 (only Thermoprobe)	Second temperature at which the NTC thermistor was calibrated. The value was measured during calibration by the manufacturer and cannot be changed.
Resistance at T2 (only Thermoprobe)	Resistance of the NTC thermistor that was measured at the 2nd temperature during calibration. The value was measured during calibration by the manufacturer and cannot be changed.
Temperature T3 (only Thermoprobe)	Third temperature at which the NTC thermistor was calibrated. The value was measured during calibration by the manufacturer and cannot be changed.

Resistance at T3 (only Thermoprobe)	Resistance of the NTC thermistor that was measured at the 3rd temperature during calibration. The value was measured during calibration by the manufacturer and cannot be changed.

Connector

The **Connector** parameter group is displayed for all digital and intelligent sensors.

Connected to	Display the measuring module or the measuring interface to which the sensor is connected.

See also

Equipment – Inventory (chapter 5.12.1, page 852)

Sensor – Definition (chapter 5.12.6, page 998)

Sensor – Status (chapter 5.12.6.3, page 1007)

User rights – Directory (chapter 4.5.7.4, page 89)

5.12.6.3 Sensor – Status

The status of a digital sensor is represented in the **Instruments** subsection as follows:

	The digital sensor is connected to the Measuring Module Digital. A measurement can be conducted.
	The digital sensor is reserved and is being used in an ongoing determination.

The monitoring status of the sensor working life and the calibration validity period is displayed as follows for analog and digital sensors in the **Sensors** subsection in the sensor list:

●	The working life of the sensor or the validity period of the calibration lies within the defined validity period.
▲	Advance warning: The working life of the sensor or the validity period of the calibration will expire after the defined advance warning time. Please observe the expiry date.

The working life of the sensor or the validity period of the calibration has expired. The sensor may not be used anymore or must be recalibrated before its next use.

See also

Enabling monitoring (chapter 5.7, page 193)

Sensor – Properties (chapter 5.12.6.2, page 1001)

5.12.6.4 pH electrode – Calibrating

General notes

Assign sensor (analog electrodes only)

pH electrodes can be calibrated with the **CAL pH** command. To accomplish this, the analog electrode to be calibrated must be assigned to the command in the **Execute with** subsection of the **Properties** window in the respective measuring module. With digital electrodes, the electrode is assigned automatically.

Calibration temperature

For a correct calibration result, the temperature of all calibration buffers used during the calibration must be kept **constant**. With the second buffer, the temperature difference to the reference temperature (temperature of the first buffer) is checked. If the temperature difference exceeds 2 °C, the calibration will be canceled. The temperature can either be determined automatically with a temperature sensor or be entered manually in the **CAL pH** command in the corresponding input field in the **Parameters** subsection of the **Properties** window.

Recognizing calibration buffers automatically

The correct buffer for the selected buffer type and the appropriate buffer value for the calibration temperature are recognized on the basis of the measured potential. If a previously measured buffer is detected in the other calibration solutions, then the calibration is canceled with an error message. The buffers used must be different.

If the pH values entered in the temperature table have different numbers of decimal places and if the calibration temperature lies between 2 such pH values, then the value is interpolated linearly and rounded to the smallest number of decimal places. Metrohm recommends defining all pH values with the same number of decimal places for custom calibration buffers.

Creating samples and subsamples

Only one calibration can be executed within a sample. A new sample must therefore be created for each calibration.

For a calibration with several subsamples, the calibration in a subsample can be canceled due to an error or by clicking on Stop. To repeat the calibration, only the subsample of the concerned buffer needs to be reset to the status **Ready**.

Calibrating with a subsample using the LOOP command

The **advantage** of this approach is that the entire calibration takes place within a determination of one subsample.

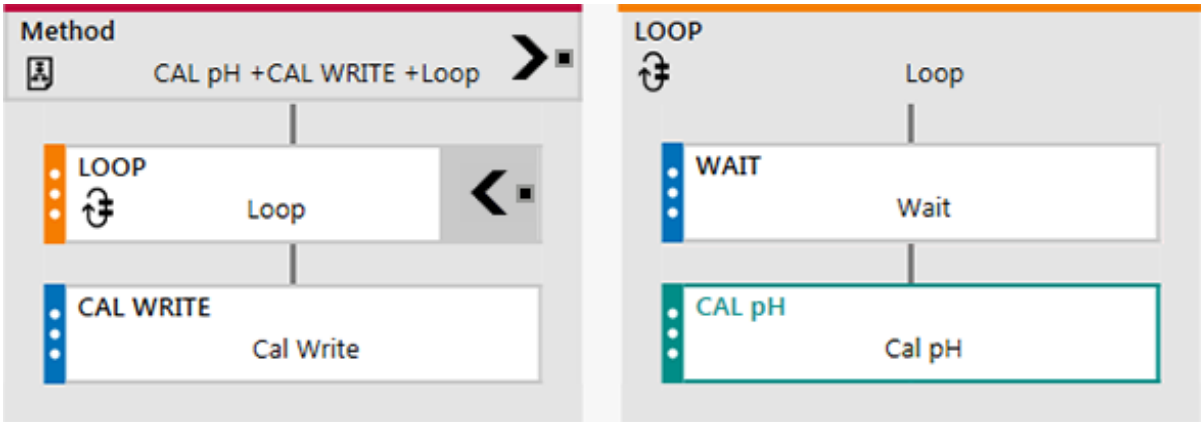


Figure 11 Example method of a calibration with a subsample using the LOOP command.

- The **CAL pH** command is in a loop and is executed according to the number of buffers.
- The calibration buffer type and the number of calibration buffers are defined in the **Parameters** subsection of the **Properties** window of the **CAL pH** command.
- Check whether the number of loop runs contained in the **LOOP** command corresponds to the defined number of calibration buffers in the **CAL pH** command.
- At the end of the calibration, the calibration data of the electrode is saved with the **CAL WRITE** command on the corresponding sensor.
- For calibration without automation, the **WAIT** command is used to interrupt the process sequence with each loop run so that the calibration buffers can be replaced manually. The message defined in the **WAIT** command must be confirmed to continue the process sequence.
- For the calibration with automation (e.g. with an **OMNIS Sample Robot**), the beakers with the buffer solutions are placed on the sample rack.
- Metrohm recommends using the provided operating procedure templates for calibration with automation (e.g. with an **OMNIS Sample Robot**). (*(see "Importing the templates", chapter 3.2, page 11)*)

Calibrating with several subsamples

The **advantage** of this approach is that each buffer solution has its own subsample data. This means that the sample position for each buffer solution can be specified in the automation with the sample robot.

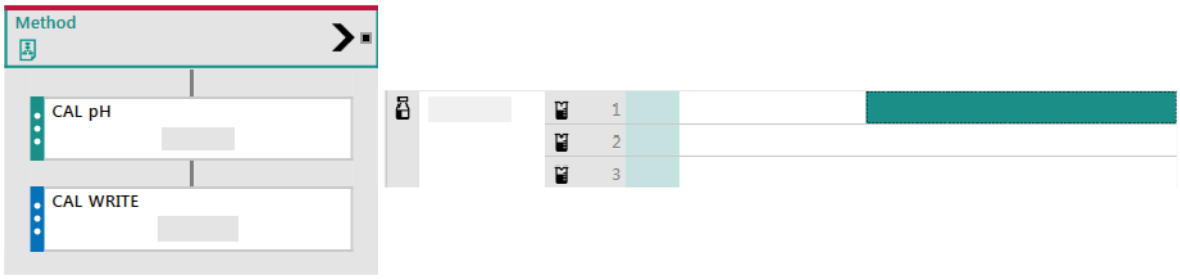


Figure 12 Example method of a calibration with multiple subsamples

- The method contains, among others, the **CAL pH** and **CAL WRITE** commands.
- The number of subsamples for the calibration within the sample must correspond to the number of buffers defined in the **CAL pH** command.
- The number of calibration buffers is defined in the **CAL pH** command. Once the required number of buffers has been measured with the same electrode, method and operating procedure within the same sample, the **CAL WRITE** command saves the calibration data of the electrode.
- For calibrations without automation, each determination is started manually as a single determination. The calibration buffer must be replaced before the start of a determination.
- Metrohm recommends using the provided operating procedure templates for calibration with automation (e.g. with an **OMNIS Sample Robot**). (*(see "Importing the templates", chapter 3.2, page 11)*)

5.12.6.5 Ion-selective electrode – Calibrating

General notes

Assigning the sensor

Ion-selective electrodes (ISE) can be calibrated with the **CAL CONC** command. To do so, the electrode to be calibrated must be assigned to the command in the **Execute with** subsection of the **Properties** window in the respective measuring module.

Defining calibration standards

For the calibration, up to 9 calibration standards can be defined in the parameters of the **CAL CONC** command. The measured value of the first 2 calibration standards has to differ by at least 6 mV. The difference for the selected unit (ppm, %, mg/L, etc.) must be 0.001 between the defined calibration standards.

Calibration temperature

For an accurate calibration result, the temperature of all the calibration standards used must be kept **constant** during the calibration. With the second standard, the temperature difference to the reference temperature (temperature of the first standard) is checked. If the temperature difference exceeds 2 °C, the calibration will be canceled. The temperature can either be determined automatically with a temperature sensor or be put in manually in the parameters of the **CAL CONC** command.

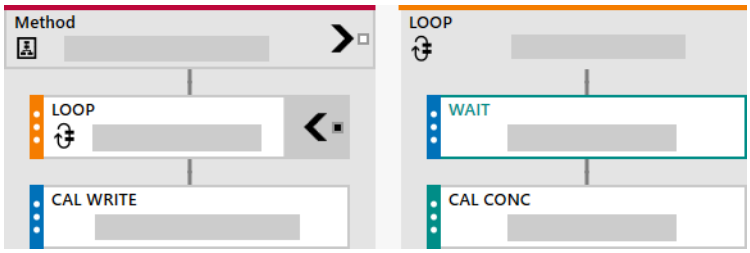
Creating samples and subsamples

Only one calibration can be executed within a sample. Therefore, create a new sample for each calibration.

For a calibration with several subsamples, the calibration in a subsample can be canceled due to an error or by pressing stop. To repeat the calibration, only the subsample of the concerned buffer has to be reset to the status **Ready**.

Calibrating with a subsample using the LOOP command

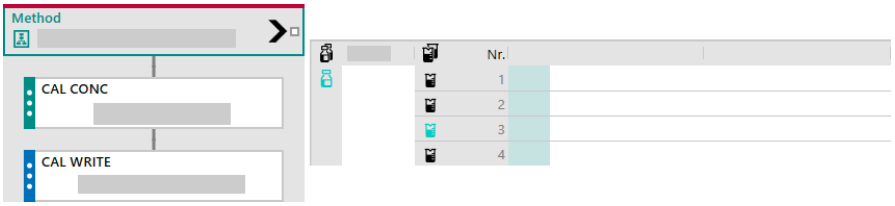
The advantage of this approach is that the entire calibration takes place within a determination of one subsample.



- The method contains, among others, the **LOOP**, **CAL CONC** and **CAL WRITE** commands.
- The **CAL CONC** command is in a loop and is executed according to the number of standards.
- The number of loop passes in the **LOOP** command must correspond to the defined number of calibration standards in the **CAL CONC** command.
- At the end of the calibration, the calibration data of the electrode is saved with the **CAL WRITE** command on the corresponding electrode.
- For the calibration without automation, the **WAIT** command is used to interrupt the method run with each loop pass so that the calibration standards can be replaced manually. The message defined in the **WAIT** command must be confirmed to continue the method run.
- For the calibration with automation (with an **OMNIS Sample Robot**), the beakers with the standard solutions must be placed on the same sample rack consecutively.

Calibrating with several subsamples

The advantage of this approach is that each standard solution has its own subsample data. This means that the sample position for each standard solution can be specified in the automation with the sample robot.



- The method contains, among others, the **CAL CONC** and **CAL WRITE** commands.
- The number of subsamples for the calibration within the sample must correspond to the number of calibration standards defined in the **CAL CONC** command.
- Once the required number of calibration standards has been measured in the same operating procedure and method and with the same work system (electrode) within the same sample, the **CAL WRITE** command saves the calibration data of the electrode.
- For calibrations without automation, each determination is started manually as a single determination. The calibration standard must be replaced before the start of a determination.

5.12.7 Solution – Definition

The term "solution" is used in the OMNIS Software for reagents which are dosed with a dosing unit. This includes titrants and auxiliary solutions. The term is also used for conductivity standards.

Additional information regarding the various solution types: *(see "Additional component – Directory", chapter 5.12.5.1, page 993)*

See also

Creating a Conductivity table (chapter 5.12.10, page 1049)

Solution – Properties (chapter 5.12.7.2, page 1014)

Solution – Status (chapter 5.12.7.3, page 1019)

5.12.7.1 Solutions – Subsection

The following functions are available in **Equipment** ▶ **Solutions**:

- **Define advance warning time** is used to define the advance warning time for the expiry date of the solutions or the titer.
- Use **Save** to save all changes.

-

  The view is reloaded with **Update view**. Unsaved entries are reset to the last saved version.
-

  Delete solutions deletes all selected solutions. If conductivity standards have been selected, then the data will be permanently deleted. The data of other solutions is retained on the memory chip.

In addition, the following windows can be opened:

-

  A template for conductivity standards is displayed in the **Inventory** window.
-

  The properties of the selected element are displayed in the **Properties** window.

Overview list

The following information is displayed in the overview list:

 	Status display of the solution. ▪ **Green icon:** The solution is connected to a cylinder unit or dosing unit. ▪ **Gray icon:** The solution is not connected to a cylinder unit or a dosing unit.
Product type	Type of solution: Single-use, multi-use, Solution IDU/IEU or conductivity standard.
Name	Name of the solution that can be modified by the user in the properties of the solution as needed (not possible with bottle cap single-use).
Connected to	Name of the cylinder unit or dosing unit to which the solution is connected.
Date of titer determination	Display of the date and time of the last titer determination by the user.
Titer expiry date	Display of the expiry date of the titer, based on the validity period that was entered. The expiry date of the titer can be set in the properties of the titer. The monitoring status of the expiry date of a titer is displayed with an icon.

Solution expiry date	Display of the expiry date of the solution, based on the opening date of the solution and the working life that was entered. The expiry date of the solution can be set in the properties of the solution. The monitoring status of the expiry date of a solution is displayed with an icon.

New solutions are detected automatically by the OMNIS Software and displayed in the overview list as soon as they have been connected for the first time.
Solutions can only be removed from the overview list if they are not connected.

See also

Enabling monitoring (chapter 5.7, page 193)

Solution – Properties (chapter 5.12.7.2, page 1014)

Solution – Status (chapter 5.12.7.3, page 1019)

5.12.7.2 Solution – Properties

Clicking on under **Equipment** ▶ **Solutions** opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 2 subsections **General** and **Specific data**.

Solution Single-Use, Solution Multi-Use and Solution IDU/IEU

General

Product information	
Product name	**Solution Single-Use**: Display the name of the solution. **Solution Multi-Use** and **Solution IDU/IEU**: Display or enter name of the solution.
Product type	Display the English designation of the solution.
Production data	
Tag ID (only single-use solution and multi-use solution)	Display the ID of the memory chip in the label of the bottle cap.

Production data	
Article number (only Solution IDU/IEU)	Display the number that unambiguously identifies the solution.
Serial number (only Solution IDU/IEU)	Display the serial number of the solution.

Specific data

Depending on the solution that has been selected, different solution data can be displayed and partly edited (depending on the product type) in this subsection.

Solution data	
Product number	**Solution Single-Use**: Display the number of the product. **Solution Multi-Use**: Display or enter the number of the product.
Product batch	**Solution Single-Use**: Display the designation of the production batch of the product. **Solution Multi-Use**: Display or enter the designation of the production batch of the product.
Aspiration tubing length (only single-use solution and multi-use solution)	Enter the length of the aspiration tubing (in cm) that is connected to the bottle cap.
Aspiration tubing diameter (only single-use solution and multi-use solution)	Enter the diameter of the aspiration tubing (in mm) that is connected to the bottle cap.

Solution data	
Solution production date	**Solution Single-Use**: Display the production date of the solution. **Solution Multi-Use**: Display the production date of the solution or or define it using the date selection feature.
Solution expiry date (manufacturer)	**Solution Single-Use**: Display the expiry date of the solution in accordance with the manufacturer specification. **Solution Multi-Use**: Display the expiry date of the solution in accordance with the manufacturer specification or define it using the date selection feature.
Concentration (only Solution IDU/IEU)	Display or enter the concentration of the solution.
Concentration unit (only Solution IDU/IEU)	Display the unit used for the concentration of the solution (in mg/L)or enter a different unit.
Solution opening date	Use the date selection feature to define the opening date on which the solution was first opened.
Working life	Enter the working life of the solution in days. Alternatively, use the date selection to define the working life.
Expiry date	Display the expiry date of the solution. The expiry date is automatically calculated using the opening date of the solution and the working life entered.
Enable monitoring	Enable monitoring of the solution. If solution monitoring is activated, the monitoring status is indicated by a colored status icon in the **Solution expiry date** table column in the solution list.
Comment	Enter a comment (optional). Comment length: max. 250 characters.

Titer data	
Titer	Enter the correction factor used for calculating the actual concentration of the titrant. Calculation formula: Original concentration x factor = actual concentration.
Unit	Enter the unit of the titer.
Absolute standard deviation	Display the absolute standard deviation of the titer.
Date of titer determination	Display the date on which the titer was determined.
Validity period	Enter the validity period of the titer in days. Alternatively, use the date selection to define the validity period.
Expiry date	Display the expiry date of the titer. The expiry date is calculated automatically using the date of the titer determination and the validity period entered.
Enable monitoring	Enable titer monitoring. If titer monitoring is activated, the monitoring status is indicated by a colored status icon in the **Titer expiry date** table column in the solution list.
Subsample ID	Display the object ID of the subsample with which the titer was written.
Number of subsamples	Display the number of subsamples that were used for determining the titer. If the titer is entered manually, then 0 is displayed for the number of subsamples.

The **Component 1** to **Component 10** parameter groups can be displayed for **Solution Single-Use** and displayed and edited for **Solution Multi-Use**.

With solutions of the **Solution Single-Use** type, components are displayed only if the manufacturer has saved backed them up on the memory chip in the label of the bottle cap.

Component 1 to Component 10	
Name	Display or enter the name of the solution component.
Molecular formula	Display or enter the molecular formula of the solution component.

Component 1 to Component 10	
Molar mass	Display or enter the molar mass of the solution component (in g/mol).
CAS Registry Number	Display or enter the registry number for the component in accordance with CAS (Chemical Abstracts Service).
Concentration	Display or enter the concentration of the component.
Concentration unit	Display the unit for the concentration of the solution (in mg/L) or enter a different unit.

The **Adsorber data** parameter group can be displayed and entered only for **Solution Single-Use** and for **Solution Multi-Use**.

Adsorber data	
Adsorber substance	Enter the type of adsorber material filled in.
Adsorber opening date	Use the date selection feature to define the opening date on which the adsorber was filled in.

Connector	
Connected to	Display the dosing unit to which the solution is connected.

- Solution data can be edited only if the respective solutions are connected to the OMNIS system with bottle cap single-use or multi-use or the **807 Dosing Unit** or the **806 Exchange Unit**.
- The data of conductivity standards can be edited at any time.
- Modified data of a solution cannot be saved as long as this solution is being used in the process sequence of a method.

Conductivity standard

Conductivity standards are defined in the **Conductivity table** subsection.

General

Product information	
Product name	Enter the name of the conductivity standard.
Product type	Display the English designation of the conductivity standard.

Specific data

Conductivity standard data	
Expiry date	Display the expiry date of the conductivity standard or define it using the date selection feature.

Conductivity table

The **Conductivity standard** can be defined in tabular form in this area. To accomplish this, a **Temperature** and the associated **Conductivity κ** must always be entered in each table line.

See also

Creating a Conductivity table (chapter 5.12.10, page 1049)

Enabling monitoring (chapter 5.7, page 193)

Sensor – Status (chapter 5.12.6.3, page 1007)

Solution – Status (chapter 5.12.7.3, page 1019)

User rights – Directory (chapter 4.5.7.4, page 89)

5.12.7.3 Solution – Status

The status of a solution is represented in the **Instruments** subsection as follows:

	The Liquid Adapter is not connected.
	The Liquid Adapter is connected, but no solution was detected.
	The Liquid Adapter is connected and a solution is connected with the bottle cap multi-use.
	The Liquid Adapter is connected and a solution is connected with the bottle cap single-use.

	The Liquid Adapter is reserved. This is used for an ongoing determination.

If the monitoring is activated, then the monitoring status of solutions and titers in the subsection **Solutions** in the solution list will be displayed as follows:

●	The titer of the solution or the working life of the solution is within the defined period of validity.
▲	The titer of the solution or the working life of the solution expires after the defined advance warning time.
■	The titer of the solution or the working life of the solution has expired.

See also

Enabling monitoring (chapter 5.7, page 193)

Solution – Definition (chapter 5.12.7, page 1012)

Solution – Properties (chapter 5.12.7.2, page 1014)

User rights – Directory (chapter 4.5.7.4, page 89)

5.12.7.4 Defining solution conditions and sensor conditions

Information on the **Solution conditions** and **Sensor conditions** in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The method must be assigned a work system with intelligent solution or digital sensor.
- The method containing the command for which a solution condition or sensor condition is defined is opened.

1 Opening the command properties

- Select the desired command in the method editor.
- Click on to open the **Properties** window.

- Select the **Execute with** subsection.

2 Open the editor for Solution conditions and Sensor conditions

- Open the editor under the desired functional unit by clicking on **Solution conditions** or **Sensor conditions**.

Solution conditions and **Sensor conditions** can be defined only for intelligent solutions and digital sensors.

3 Selecting logical connective

Select a logical connective from the selection list:

- **All conditions must be met**
  - Only the solutions and sensors are used to which all selected conditions apply.
- **At least one condition must be met**
  - The solutions and sensors used are those to which at least one of the conditions applies.

If both **Solution conditions** and **Sensor conditions** are defined, then the Equipment to be used must meet conditions from both categories to be able to execute the command.

4 Adding Solution conditions and Sensor conditions

- Add a new condition by clicking on .

Any number of conditions can be added.

5 Select the Attribute of the condition

- Select a **Attribute** of the condition.

6 Defining the Attribute of the condition

- Select a search operator from the selection list, if necessary:
  - **Is**
    Finds the solutions and sensors for which the value in the defined condition corresponds exactly with the input.
  - **Is less than**
    Finds the solutions and sensors for which the value in the defined condition is smaller than the input.
  - **Is less than or equal to**
    Finds the solutions and sensors for which the value in the defined condition is smaller than the input or the same as the input.
  - **Is greater than**
    Finds the solutions and sensors for which the value in the defined condition is larger than the input.
  - **Is greater than or equal to**
    Finds the solutions and sensors for which the value in the defined condition is larger than the input or the same as the input.
- Then enter a value.
  If no selection list with search operators is displayed, then the required value for the **Attribute** of the condition can be entered directly.

When defining the conditions for **Solution name**, **Sensor name** and **Article number**, the character * can be used as a wildcard. This wildcard can replace a single character as well as a character string and can be used at any position.

7 Removing Solution conditions and Sensor conditions

- Remove the condition by clicking on .

8 Saving Solution conditions and Sensor conditions

- Changes are saved by clicking on .

The number of saved **Solution conditions** and **Sensor conditions** is displayed in the **Execute with** subsection.

A command containing the **solution conditions** or **sensor conditions** is marked with in the method editor and operating procedures editor. A method containing a command with **solution condi-**

tions or **sensor conditions** is indicated with in the operating procedures editor.

Solution conditions and **Sensor conditions** are defined according to the command for the assigned functional unit of the work system and stored in the method. In another method, different **Solution conditions** and **Sensor conditions** can be defined for the same command.

If the conditions are to be taken into account when executing the operating procedure or method, then the assigned **Work system** must be used. If the original **Work system** is replaced by another **Work system**, then the defined **Solution conditions** and **Sensor conditions** are lost.

See also

Assigning a functional unit to a command (chapter 5.12.3.3, page 905)

5.12.8 Sample rack – Definition

A sample rack is used for the storage of sample vessels and is placed on the rack base of the sample robot or on the turntable of the sample changer.

Additional information regarding the various sample rack types: *(see "Additional component – Directory", chapter 5.12.5.1, page 993)*

See also

Sample rack – Properties (chapter 5.12.8.2, page 1025)

Sample rack – Status (chapter 5.12.8.3, page 1030)

5.12.8.1 Sample racks – Subsection

The following functions are available under **Equipment** ▶ **Sample racks**:

- Use **Import rack definitions** to import rack definitions for customized sample racks from XML files.
- Use **Save** to save all changes.
- The view is reloaded with **Update view**. Unsaved entries are reset to the last saved version.

-

  Use **Remove sample racks** to remove all selected sample racks. If a **OMNIS Sample Rack** is removed, then the data is retained on the memory chip of the sample rack. If a **Sample Processor Rack** is removed, then the data saved in the OMNIS Software is deleted. New data will be stored if the sample rack is used again.

In addition, the following window can be opened:

-

  The properties of the selected element are displayed in the **Properties** window.

Overview list

The following information is displayed in the overview list:

 	Status display of the sample rack. ▪ **Green icon**: The sample rack is placed on either the rack base of the sample robot or the turntable of the sample changer. ▪ **Gray icon**: The sample rack is not placed on either the rack base of the sample robot or the turntable of the sample changer.
Product type	Type of the product.
Name	Name of the sample rack.
Placed on	Sample robot or sample changer on which the sample rack is placed.
Position	Position of the sample rack on the sample robot.
Number of positions	Number of positions for samples on the rack.

New sample racks are detected automatically by the OMNIS Software and displayed in the overview list as soon as sample racks have been placed for the first time on the rack base of the sample robot or on the turntable of the sample changer. In order for a **Sample Processor Rack** to be detected, the sample changer needs to be reinitialized in addition after the sample rack has been set in place. As long as a sample rack is in place, it cannot be removed from the overview list.

If a sample rack is disconnected from the rack base or the turntable, it continues to be visible in the overview list, but its properties can no longer be edited.

See also

Sample rack – Properties (chapter 5.12.8.2, page 1025)

5.12.8.2 Sample rack – Properties

Clicking on under **Equipment** ▶ **Sample racks** opens the **Properties** window. Depending on the selected element, the following functions and information are available in the 3 subsections **General**, **Specific data** and **Positions on the rack**:

If a **Sample Processor Rack** is selected, rack parameters for the selected sample rack can be imported by clicking on . All the editable parameters in the properties of the selected sample rack are imported. Additional information on importing rack parameters: *(see "Importing rack parameters", chapter 5.12.8.5, page 1032)*
The rack parameters of the selected **Sample Processor Rack** can be exported by clicking on . All the editable parameters in the properties of the selected sample rack are exported. Additional information on exporting rack parameters: *(see "Exporting rack parameters", chapter 5.12.8.6, page 1033)*

General

Product information	
Product name	**OMNIS Sample Rack**: Display or enter the name of the sample rack. The name is saved on the memory chip of the sample rack. **Sample Processor Rack**: Display the name of the sample rack. The name is generated automatically from the article number of the sample rack and the serial number of the sample changer used and is saved on the local computer. The name cannot be edited.
Product type	Show the English designation of the sample rack.
Production data	
Article number	Show the number that unambiguously identifies the sample rack.
Serial number (only OMNIS Sample Rack)	Display the serial number of the sample rack.

Specific data

Rack data	
Number of positions	Display the number of positions of the sample rack.
Vessel diameter (only OMNIS Sample Rack)	Display the diameter (in mm) of the sample vessel.
Vessel height (only OMNIS Sample Rack)	Display the height (in mm) of the sample vessel.
Rack code (only Sample Processor Rack)	Display the magnet code for identifying the rack (with the article number).
Rack offset (only Sample Processor Rack)	Enter the offset value of the rack (in °). The rack offset is a production-related tolerance between the upper and lower section of the rack. The value of the rack offset is determined with a rack adjustment by the regional Metrohm service representative.
Vessel sensor (only Sample Processor Rack of 874 Oven Sample Processor)	Select or deactivate the vessel sensor. After a position on the sample rack has been approached with a **MOVE TO RACK** command or in the manual control, the vessel sensor checks if a sample vessel is present at the selected position. ▪ **Tower**: Activate the vessel sensor installed in the tower. Only positions on single-row sample racks can be checked. ▪ **Off**: Disable vessel sensor. **Note**: This parameter is identical with the **beaker sensor** parameter used in previous Metrohm applications. The designation **Vessel sensor** in the OMNIS Software corresponds to the designation **beaker sensor** used in the product manual.
Placement	
Placed on	Display the sample robot or sample changer on the rack base or turntable of which the sample rack is mounted.

Positions on the rack

The **Positions on the rack** subsection is available only under **Equipment** ▶ **Sample racks** for instruments of the **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler** types.

For the 1-tower version of sample changers, the settings of the **Tower 1** parameter group are read out.

Sample positions	
Vessel sensor	Select or disable the vessel sensor. After a position on the sample rack has been approached with a **MOVE TO RACK** command or in the manual control, the vessel sensor checks if a sample vessel is present at the selected position. ▪ **Tower**: Activate the vessel sensor installed in the tower. Only positions on single-row sample racks can be checked. ▪ **Robotic arm**: If a robotic arm with built-in vessel sensor is used, it can be activated here. After approaching the position on the sample rack, the lift is additionally moved to the work height. The work height must be defined in such a way that there is contact between the robotic arm and the sample vessel. ▪ **Off**: Disable vessel sensor. **Note**: ▪ This vessel sensor selection applies only for sample positions. The vessel sensor can be specifically enabled or disabled for each special position. ▪ This parameter is identical to the **beaker sensor** parameter used in previous Metrohm applications. The **Vessel sensor** designation in the OMNIS Software corresponds to the **beaker sensor** designation used in the product manual.

Tower 1 / Tower 2	
Work height	Enter the height (in mm) that the lift is to move to when executing a determination. The electrodes, stirrers and buret tips are positioned at this lift position for analysis. **Note**: This work height only applies for sample positions. A separate work height can be defined for each special position and each external position. Additional information on defining lift heights: *(see "Defining the lift height", chapter 5.12.3.30.3, page 978)*
Rinse height	Enter the height (in mm) that the lift is to move to for rinsing. The electrodes, stirrers and buret tips are positioned at this lift position for cleaning. **Note**: This rinse height only applies for positions on the rack. The rinse height for external positions can be defined in the properties of the 786 Swing Head. Additional information on defining lift heights: *(see "Defining the lift height", chapter 5.12.3.30.3, page 978)*
Change height	Enter the height (in mm) that the lift is to move to for the rotating movement of the sample rack or the swing movement of the robotic arm when changing the position on the rack. The collision of electrodes, stirrers or buret tips with sample vessels is prevented at this lift position. If the lift is at a lower lift height than the change height before the rotating movement of the sample rack or the swing movement of the robotic arm, then the lift is automatically moved to the change height. If the lift is at a higher lift height than the change height, the rotating movement or swing movement is carried out at the current lift height. **Note**: The change height only applies for positions on the rack. For external positions, the swing height that can be defined in the properties of the 786 Swing Head is used. Further information on defining lift heights: *(see "Defining the lift height", chapter 5.12.3.30.3, page 978)*

Tower 1 / Tower 2	
Special height	Enter the special height (in mm) that can be used, for example to immerse a pipetting tip. **Note**: The special height only applies for positions on the rack.

A **special position** can be added by clicking :*(see "Defining a special position", chapter 5.12.3.30.4, page 982)*

Special position	
Position	Enter the position on the sample rack that is defined as special position. This position cannot be defined as sample position anymore in the subsample data.
Vessel sensor	Selecting or disabling the vessel sensor (*see above*). **Note**: ▪ The vessel sensor can be specifically selected or deactivated for each special position. For sample positions, the vessel sensor can be selected or disabled in the same subsection in the **Sample positions** parameter group. ▪ This parameter is identical with the **beaker sensor** parameter used in previous Metrohm applications. The **Vessel sensor** designation in the OMNIS Software corresponds to the **beaker sensor** designation used in the product manual.

Tower 1 / Tower 2	
Work height	Enter the work height (in mm) that the lift should move to for the special position when executing a determination. The electrodes, stirrers and buret tips are positioned at this lift position for analysis. **Note**: A separate work height can be defined for each special position. The work height for sample positions can be defined in the same subsection in the lift heights for all positions on the rack.

The **Rinse height**, the **Change height** and the **Special height** apply for all positions on the sample rack, i.e. for sample positions as well as special positions.

See also

Defining a special position (chapter 5.12.3.30.4, page 982)

Defining the lift height (chapter 5.12.3.30.3, page 978)

Exporting rack parameters (chapter 5.12.8.6, page 1033)

Importing rack parameters (chapter 5.12.8.5, page 1032)

Sample rack – Definition (chapter 5.12.8, page 1023)

Sample rack – Status (chapter 5.12.8.3, page 1030)

User rights – Directory (chapter 4.5.7.4, page 89)

5.12.8.3 Sample rack – Status

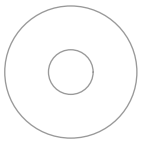
The status of the sample racks is represented in the **Instruments** subsection as follows:

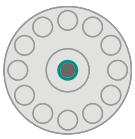
Table 8 OMNIS Sample Robot, OMNIS Sample Robot NIR and OMNIS Sample Robot Oven

	No sample rack has been placed on the rack base.
	A sample rack has been placed on the rack base. The name of the sample rack is displayed in the tooltip.
	A sample rack has been placed on the rack base. Samples of this sample rack are currently being analyzed.
	A sample rack has been placed on the rack base. Samples of this sample rack are currently awaiting analysis.

A sample rack that is used in the determination run or that is waiting for the execution of the determination must not be removed from the rack base.

Table 9 814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler and 874 Oven Sample Processor

	No sample rack has been placed on the turntable or the magnet code of the mounted sample rack has not yet been read by initializing the sample changer.



A sample rack has been placed on the turntable. The name of the sample rack is displayed in the tooltip.

See also

Additional component – Directory (chapter 5.12.5.1, page 993)

5.12.8.4 Importing rack definitions

In order for customized sample racks to be used by the OMNIS Software, their rack definitions must be imported into the OMNIS Software. After importing the rack definitions according to these instructions, placing the corresponding sample racks on the sample changers, and initializing the instrument, the sample racks will appear in the **Sample racks** subsection.

Prerequisite:

- At least one rack definition is available as an XML file.
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting rack definitions

- Click on to open the **Import rack definition** window under **Equipment** ▶ **Sample racks**.

2 Browsing for folders

- Select the folder in which the desired rack definitions are saved.

3 Selecting files

- Select the rack definition files or enter the name of a rack definition file in the **File name** field.

4 Confirming and importing the selection

- Click **[Open]** to confirm the selection.

The rack definitions have been imported into the OMNIS Software. The corresponding sample racks will appear in the **Sample racks** subsection once they have been placed on the sample changer and the instrument has been initialized.

If the rack code of the rack definitions to be imported is invalid or already exists in a rack definition in the OMNIS Software, then the **Rack code invalid or already exists** dialog will open. The rack names and the rack codes for the sample racks can be redefined in the dialog.

Customized sample racks are not recognized automatically by the OMNIS Software when reserving the sample changer. In order for the sample racks in place to be recognized by the OMNIS Software, the sample changer or the **Tower** functional unit must be reinitialized afterwards.

See also

Sample rack – Definition (chapter 5.12.8, page 1023)

Sample rack – Properties (chapter 5.12.8.2, page 1025)

Sample racks – Subsection (chapter 5.12.8.1, page 1023)

5.12.8.5 Importing rack parameters

Rack parameters can be imported for sample racks of the **Sample Processor Rack** type of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**. All the editable parameters in the properties of the selected sample rack are imported.

Prerequisite:

- A sample rack is in place and has been detected.
- At least one OMNIS rack configuration file (***.orco**) is available.
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting the rack parameter

- Select the required sample rack under **Equipment** ▶ **Sample racks** and open the **Properties** window by clicking on .
  or
  Select the required sample rack under **Equipment** ▶ **Instruments** and open the **Properties** window by clicking on .
- Open the **Import rack parameters** window by clicking on in the **Properties** window.

Rack parameters can only be imported for sample racks that are placed on the turntable of the sample changer and have been recognized by the OMNIS Software.

2 Browsing for folder

- Select the folder in which the desired rack parameter is saved.

3 Selecting the file

- Select the OMNIS rack configuration file or enter the name of the OMNIS rack configuration file in the **File name** field.

4 Confirming and importing the selection

- Click **[Open]** to confirm the selection.

The rack parameters for the selected sample rack are imported into the OMNIS Software.

See also

Exporting rack parameters (chapter 5.12.8.6, page 1033)

Sample rack – Properties (chapter 5.12.8.2, page 1025)

5.12.8.6 Exporting rack parameters

The rack parameters of sample racks of the **Sample Processor Rack** type of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler** can be exported. All the editable parameters in the properties of the selected sample rack are exported.

Prerequisite:

- A sample rack is in place and has been detected.
- The user has the necessary rights. Further information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Exporting rack parameters

- Select the required sample rack under **Equipment** ▶ **Sample racks** and open the **Properties** window by clicking on .
  or
  Select the required sample rack under **Equipment** ▶ **Instruments** and open the **Properties** window by clicking on .
- Open the **Export rack parameters** window by clicking on in the **Properties** window.

Only rack parameters of sample racks that are placed on the turntable of the sample changer and have been recognized by the OMNIS Software can be exported.

2 Selecting or entering a target folder

- Select the target folder or enter the absolute path in the address bar where the exported file is to be saved.

3 Defining a file name (optional)

- Enter the name under which the file is to be saved in the **File name** field.

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

4 Creating a file

- Create the file by clicking on **[Save]**.

The rack parameters are exported as a file to the selected folder.

Regardless of the rack type, the exported rack parameters can be imported and used for every **Sample Processor Rack** of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**.

All time indications are converted into the Coordinated Universal Time (UTC±00:00) when exporting. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.
For the date and time displayed in the file name, the local time on the computer is used.

See also

Importing rack parameters (chapter 5.12.8.5, page 1032)

Sample rack – Properties (chapter 5.12.8.2, page 1025)

5.12.9 Calibration buffers – Definition

Calibration buffers are used to calibrate pH electrodes with the help of the **CAL pH** command. The slope and the electrode zero point are determined at this time. Not only **customized calibration buffers** but also the **commercial calibration buffers** stored in the system can be used.

Custom calibration buffers

In the **Custom calibration buffers** subsection, a maximum of nine custom calibration buffers can be defined and edited for pH calibration. The buffer recognition proceeds automatically.

Commercial calibration buffers

Predefined, commercially available buffer series are available in the system. The following buffer series can be selected as a buffer type in the **CAL pH** command:

- **Metrohm**
- **Baker**
- **Beckman**
- **DIN**
- **Fisher**
- **Fluka**
- **Hamilton DURACAL**
- **Merck CertiPUR 20 / Titrisol**
- **Merck CertiPUR 25**
- **Mettler Toledo**
- **NIST**
- **Radiometer Analytical**

See also

Baker buffer type (chapter 5.12.9.3, page 1039)

Beckmann buffer type (chapter 5.12.9.4, page 1040)

Buffer type Merck CertiPUR 25 (chapter 5.12.9.10, page 1046)

CAL pH – Properties (chapter 5.11.8.32, page 679)

DIN buffer type (in accordance with DIN standard 19267, 2012) (chapter 5.12.9.5, page 1041)

Editing custom calibration buffers (chapter 5.12.9.1.1, page 1036)

Fisher buffer type (chapter 5.12.9.6, page 1042)

Fluka buffer type (chapter 5.12.9.7, page 1043)

Hamilton DURACAL buffer type (chapter 5.12.9.8, page 1044)

Merck CertiPUR 20/Titrisol buffer type (chapter 5.12.9.9, page 1045)

Metrohm buffer type (chapter 5.12.9.2, page 1038)

Mettler Toledo buffer type (chapter 5.12.9.11, page 1046)

NIST buffer type (chapter 5.12.9.12, page 1047)

Radiometer Analytical buffer type (chapter 5.12.9.13, page 1048)

pH electrode – Calibrating (chapter 5.12.6.4, page 1008)

5.12.9.1 Custom calibration buffers – Subsection

The following functions are available in **Equipment** ▶ **Custom calibration buffers**:

-

  Create temperature table is used to create a new temperature table for an additional custom calibration buffer.
-

  Use **Save** to save all changes.
-

  The view is reloaded with **Update view**. Unsaved entries are reset to the last saved version.

In addition, the designation for the type of the custom calibration buffer can be entered via the **Name of the buffer type** field.

See also

Editing custom calibration buffers (chapter 5.12.9.1.1, page 1036)

5.12.9.1.1 Editing custom calibration buffers

A maximum of 9 custom calibration buffers can be defined and edited in the **Equipment** work area under **Custom calibration buffers**. By default, 2 empty temperature tables for buffers are already available.

Proceed as follows to edit the temperature tables for the buffers:

1 Opening the subsection

- In the **Equipment** work area, click on **Custom calibration buffers**.

The **Custom calibration buffers** subsection opens, in which 2 empty temperature tables for buffers have been created by default.

2 Entering a name

- Enter the required name for the custom buffer type in the **Name of the buffer type** field.

3 Filling in a temperature table

- Fill in temperature tables with pH values as needed (permitted range: pH -20 to +20).

If the pH values entered in the temperature table have different numbers of decimal places and if the calibration temperature lies between 2 such pH values, then the value is interpolated linearly and rounded to the smallest number of decimal places. Metrohm recommends defining all pH values with the same number of decimal places for custom calibration buffers.

4 Creating a new temperature table

- If needed, create more temperature tables by clicking on .

5 Deleting a temperature table

- To delete a temperature table that is no longer required, right-click in a table field and select **[Delete buffer]**. All temperature tables except for 2 can be deleted.

6 Saving temperature tables

- Save temperature tables of the custom calibration buffers by clicking on the icon.

For custom calibration buffers, enter at a minimum the pH values for the temperature range in which the pH calibration and pH measurement will be carried out later.

See also

Baker buffer type (chapter 5.12.9.3, page 1039)

Beckmann buffer type (chapter 5.12.9.4, page 1040)

Buffer type Merck CertiPUR 25 (chapter 5.12.9.10, page 1046)

Calibration buffers – Definition (chapter 5.12.9, page 1034)

DIN buffer type (in accordance with DIN standard 19267, 2012) (chapter 5.12.9.5, page 1041)

Fisher buffer type (chapter 5.12.9.6, page 1042)

Fluka buffer type (chapter 5.12.9.7, page 1043)

Hamilton DURACAL buffer type (chapter 5.12.9.8, page 1044)

Merck CertiPUR 20/Titrisol buffer type (chapter 5.12.9.9, page 1045)

Metrohm buffer type (chapter 5.12.9.2, page 1038)

Mettler Toledo buffer type (chapter 5.12.9.11, page 1046)

NIST buffer type (chapter 5.12.9.12, page 1047)

Radiometer Analytical buffer type (chapter 5.12.9.13, page 1048)

5.12.9.2 Metrohm buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

Metrohm buffer solutions

Temp. (°C)	pH 4.00	pH 7.00	pH 9.00
0	3.99	7.11	9.27
5	3.99	7.08	9.18
10	3.99	7.06	9.13
15	3.99	7.04	9.08
20	3.99	7.02	9.04
25	**4.00**	**7.00**	**9.00**
30	4.00	6.99	8.96
35	4.01	6.98	8.93
40	4.02	6.98	8.90
45	4.03	6.97	8.87
50	4.04	6.97	8.84
55	4.06	6.97	8.81
60	4.07	6.97	8.79
65	4.09	6.98	8.76
70	4.11	6.98	8.74
75	4.13	6.99	8.73
80	4.15	7.00	8.71
85	4.18	7.00	8.70
90	4.20	7.01	8.68
95	4.23	7.02	8.67

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.3 Baker buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

pH values represented in *italics* are interpolated or extrapolated values. The other values correspond to the manufacturer's specifications.

Baker buffer solutions

Temp. (°C)	pH 4.00	pH 7.00	pH 9.00	pH 10.00
0	4.00	7.13	9.23	10.30
5	*4.00*	*7.09*	*9.17*	*10.24*
10	4.00	7.05	9.10	10.17
15	*4.00*	*7.03*	*9.05*	*10.11*
20	**4.00**	**7.00**	**9.00**	10.05
25	*4.00*	*6.98*	*8.96*	**10.00**
30	4.01	6.98	8.91	9.96
35	*4.02*	*6.98*	*8.88*	*9.93*
40	4.03	6.97	8.84	9.89
45	*4.04*	*6.97*	*8.81*	*9.86*
50	4.05	6.96	8.78	9.82
55	*4.07*	*6.96*	*8.76*	*9.79*
60	4.08	6.96	8.73	9.76
65	*4.10*	*6.97*	*8.71*	*9.74*
70	4.12	6.97	8.69	9.72
75	*4.14*	*6.98*	*8.68*	*9.70*
80	4.16	6.98	8.66	9.68
85	*4.19*	*6.99*	*8.64*	*9.66*
90	4.21	7.00	8.62	9.64
95	-	-	-	-

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.4 Beckmann buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

Beckmann buffer solutions

Temp. (°C)	pH 4.000	pH 7.000	pH 10.010
0	4.000	7.120	10.320
5	4.000	7.090	10.250
10	4.000	7.060	10.180
15	4.000	7.040	10.120
20	4.000	7.020	10.060
25	**4.000**	**7.000**	**10.010**
30	4.010	6.990	9.970
35	4.020	6.985	9.930
40	4.030	6.980	9.890
45	4.045	6.975	9.860
50	4.060	6.970	9.830
55	4.075	6.975	-
60	4.090	6.980	-
65	4.105	6.985	-
70	4.120	6.995	-
75	4.140	7.000	-
80	4.160	7.000	-
85	4.175	7.010	-
90	4.190	7.02	-
95	4.210	7.030	-

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.5 DIN buffer type (in accordance with DIN standard 19267, 2012)

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

pH values represented in *italics* are interpolated or extrapolated values. The other values correspond to the manufacturer's specifications.

DIN buffer solutions

Temp. (°C)	pH 1.09	pH 3.06	pH 4.65	pH 6.79	pH 9.23	pH 12.75
0	1.08	-	4.67	6.89	9.48	-
5	*1.08*	-	*4.66*	*6.86*	*9.43*	-
10	1.09	3.10	4.66	6.84	9.37	13.37
15	*1.09*	*3.08*	*4.65*	*6.82*	*9.32*	*13.15*
20	1.09	3.07	4.65	6.80	9.27	12.96
25	**1.09**	**3.06**	**4.65**	**6.79**	**9.23**	**12.75**
30	1.10	3.05	4.65	6.78	9.18	12.61
35	*1.10*	*3.05*	*4.66*	*6.77*	*9.13*	*12.44*
40	1.10	3.04	4.66	6.76	9.09	12.29
45	*1.10*	*3.04*	*4.67*	*6.76*	*9.04*	*12.13*
50	1.11	3.04	4.68	6.76	9.00	11.98
55	*1.11*	*3.04*	*4.69*	*6.76*	*8.97*	*11.84*
60	1.11	3.04	4.70	6.76	8.92	11.69
65	*1.11*	*3.04*	*4.71*	*6.76*	*8.90*	*11.56*
70	1.11	3.04	4.72	6.76	8.88	11.43
75	*1.12*	*3.04*	*4.74*	*6.77*	*8.86*	*11.30*
80	1.12	3.05	4.75	6.78	8.85	11.19
85	*1.12*	*3.06*	*4.77*	*6.79*	*8.83*	*11.08*
90	1.13	3.07	4.79	6.80	8.82	10.99
95	-	-	-	-	-	-

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.6 Fisher buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

pH values represented in *italics* are interpolated or extrapolated values. The other values correspond to the manufacturer's specifications.

Fisher buffer solutions

Temp. (°C)	pH 2.00	pH 4.00	pH 7.00	pH 10.00
0	-	4.01	7.13	10.34
5	1.98	3.99	7.10	10.26
10	1.98	4.00	7.07	10.19
15	2.02	3.99	7.05	10.12
20	2.00	4.00	7.02	10.06
25	**2.00**	**4.00**	**7.00**	**10.00**
30	2.00	4.01	6.99	9.94
35	2.02	4.02	6.98	9.90
40	2.01	4.03	6.97	9.85
45	2.01	*4.04*	*6.97*	*9.81*
50	2.01	4.06	6.97	9.78
55	-	*4.07*	*6.97*	*9.74*
60	-	4.09	6.98	9.70
65	-	*4.11*	*6.99*	*9.68*
70	-	*4.13*	*7.00*	*9.65*
75	-	*4.14*	*7.02*	*9.63*
80	-	*4.16*	*7.03*	*9.62*
85	-	*4.18*	*7.06*	*9.61*
90	-	*4.21*	*7.08*	*9.60*
95	-	*4.23*	*7.11*	*9.60*

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.7 Fluka buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

pH values represented in *italics* are interpolated or extrapolated values. The other values correspond to the manufacturer's specifications.

Fluka buffer solutions

Temp. (°C)	pH 4.000	pH 7.000	pH 9.000
0	4.030	7.130	9.240
5	4.025	7.090	9.175
10	4.020	7.050	9.110
15	4.010	7.020	9.055
20	**4.000**	**7.000**	**9.000**
25	4.000	6.990	8.965
30	4.000	6.980	8.930
35	4.000	6.975	8.895
40	4.000	9.970	8.860
45	4.000	6.965	8.830
50	4.000	6.960	8.800
55	4.000	6.960	8.775
60	4.000	6.960	8.750
65	4.000	*6.965*	*8.730*
70	4.000	6.970	8.710
75	4.000	*6.975*	*8.690*
80	4.000	6.980	8.670
85	4.000	*6.990*	*8.655*
90	4.000	7.000	8.640
95	4.000	*7.010*	*8.620*

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.8 Hamilton DURACAL buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

Hamilton DURACAL buffer solutions

Temp. (°C)	pH 4.01	pH 7.00	pH 9.21	pH 10.01
0	0	0	0	0
5	4.01	7.09	9.45	10.19
10	4.00	7.06	9.38	10.15
15	4.00	7.04	9.32	10.11
20	4.00	7.02	9.26	10.06
25	**4.01**	**7.00**	**9.21**	**10.01**
30	4.01	6.99	9.16	9.97
35	4.02	6.98	9.11	9.92
40	4.03	6.97	9.06	9.86
45	4.04	6.97	9.03	9.83
50	4.06	6.97	8.99	9.79
55	-	-	-	-
60	-	-	-	-
65	-	-	-	-
70	-	-	-	-
75	-	-	-	-
80	-	-	-	-
85	-	-	-	-
90	-	-	-	-
95	-	-	-	-

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.9 Merck CertiPUR 20/Titrisol buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

pH values represented in *italics* are interpolated or extrapolated values. The other values correspond to the manufacturer's specifications.

Merck CertiPUR 20 / Titrisol buffer solutions

Temp. (°C)	pH 2.000	pH 4.000	pH 7.000	pH 9.000	pH 12.000
0	2.010	4.050	7.130	9.240	12.580
5	2.010	4.040	7.070	9.160	12.410
10	2.010	4.020	7.050	9.110	12.260
15	2.000	4.010	7.020	9.050	12.100
20	**2.000**	**4.000**	**7.000**	**9.000**	**12.000**
25	2.000	4.010	6.980	8.950	11.880
30	2.000	4.010	6.980	8.910	11.720
35	2.000	4.010	6.960	8.880	11.670
40	2.000	4.010	6.950	8.850	11.540
45	*2.000*	*4.000*	*6.950*	*8.820*	*11.435*
50	2.000	4.000	6.950	8.790	11.330
55	*2.000*	*4.000*	*6.950*	*8.760*	*11.185*
60	2.000	4.000	6.960	8.730	11.040
65	*2.000*	*4.000*	*6.960*	*8.715*	*10.970*
70	2.010	4.000	6.960	8.700	10.900
75	*2.010*	*4.000*	*6.960*	*8.680*	*10.800*
80	2.010	4.000	6.970	8.660	10.700
85	*2.010*	*4.000*	*6.980*	*8.650*	*10.590*
90	2.010	4.000	7.000	8.640	10.480
95	-	*4.000*	*7.020*	-	-

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible. However, they may be changed by the respective manufacturers.

The CertiPUR 20 and Titrisol product lines have the identical values.

5.12.9.10 Buffer type Merck CertiPUR 25

Merck CertiPUR 25 buffer solutions

Temp. (°C)	pH 4.00	pH 7.00	pH 9.00	pH 10.00
0	-	-	-	-
5	4.05	7.09	9.22	10.22
10	4.04	7.06	9.16	10.18
15	4.02	7.04	9.10	10.10
20	4.01	7.02	9.05	10.05
25	**4.00**	**7.00**	**9.00**	**10.00**
30	3.99	6.98	8.96	9.94
35	3.98	6.98	8.93	9.90
40	3.98	6.97	8.89	9.86
45	3.98	6.97	8.86	9.80
50	3.98	6.97	8.84	9.73
55	-	-	-	-
60	-	-	-	-
65	-	-	-	-
70	-	-	-	-
75	-	-	-	-
80	-	-	-	-
85	-	-	-	-
90	-	-	-	-
95	-	-	-	-

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.11 Mettler Toledo buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

pH values represented in *italics* are interpolated or extrapolated values. The other values correspond to the manufacturer's specifications.

Mettler Toledo buffer solutions

Temp. (°C)	pH 2.00	pH 4.01	pH 7.00	pH 9.21	pH 11.00
0	*2.03*	*4.01*	**7.12**	*9.52*	*11.90*
5	2.02	4.01	7.09	9.45	11.72
10	2.01	4.00	7.06	9.38	11.54
15	2.00	4.00	7.04	9.32	11.36
20	2.00	4.00	7.02	9.26	11.18
25	**2.00**	**4.01**	**7.00**	**9.21**	**11.00**
30	1.99	4.01	6.99	9.16	10.82
35	1.99	4.02	6.98	9.11	10.64
40	1.98	4.03	6.97	9.06	10.46
45	1.98	4.04	6.97	9.03	10.28
50	1.98	4.06	6.97	8.99	10.10
55	*1.98*	*4.08*	*6.98*	*8.96*	-
60	*1.98*	*4.10*	*6.98*	*8.93*	-
65	*1.98*	*4.13*	*6.99*	*8.90*	-
70	*1.99*	*4.16*	*7.00*	*8.88*	-
75	*1.99*	*4.19*	*7.02*	*8.85*	-
80	*2.00*	*4.22*	*7.04*	*8.83*	-
85	*2.00*	*4.26*	*7.06*	*8.81*	-
90	*2.00*	*4.30*	*7.09*	*8.79*	-
95	-	*4.35*	*7.12*	*8.77*	-

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.12 NIST buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

pH values represented in *italics* are interpolated or extrapolated values. The other values correspond to the manufacturer's specifications.

NIST buffer solutions

Temp. (°C)	pH 1.680	pH 4.008	pH 6.865	pH 9.184	pH 12.454
0	-	4.010	6.984	9.464	13.423
5	1.668	4.004	6.950	9.392	13.207
10	1.670	4.001	6.922	9.331	13.003
15	1.672	4.001	6.900	9.277	12.810
20	1.676	4.003	6.880	9.228	12.627
25	**1.680**	**4.008**	**6.865**	**9.184**	**12.454**
30	1.685	4.015	6.853	9.144	12.289
35	1.691	4.025	6.843	9.107	12.133
40	1.697	4.036	6.837	9.076	11.984
45	1.704	4.049	6.834	9.046	11.841
50	1.712	4.064	6.833	9.018	11.705
55	1.715	4.075	6.834	8.985	11.574
60	1.723	4.091	6.836	8.962	11.449
65	*1.732*	*4.108*	*6.840*	*8.941*	-
70	1.743	4.126	6.845	8.921	-
75	*1.754*	*4.145*	*6.852*	*8.902*	-
80	1.766	4.164	6.859	8.885	-
85	*1.778*	*4.185*	*6.867*	*8.867*	-
90	1.792	4.205	6.877	8.850	-
95	1.806	4.227	6.886	8.833	-

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.9.13 Radiometer Analytical buffer type

pH values printed in **bold** are the values at the reference temperature of the respective buffer solution.

Radiometer Analytical buffer solutions

Temp. (°C)	pH 1.679	pH 4.005	pH 7.000	pH 9.180
0	1.666	4.000	7.118	9.464
5	1.668	3.998	7.087	9.395

Temp. (°C)	pH 1.679	pH 4.005	pH 7.000	pH 9.180
10	1.670	3.997	7.059	9.332
15	1.672	3.998	7.036	9.276
20	1.675	4.001	7.016	9.225
25	**1.679**	**4.005**	**7.000**	**9.180**
30	1.683	4.011	6.987	9.139
35	1.688	4.018	6.977	9.102
40	1.694	4.027	6.970	9.068
45	1.700	4.038	6.965	9.038
50	1.707	4.050	6.964	9.011
55	1.715	4.064	6.965	8.985
60	1.723	4.080	6.968	8.962
65	1.732	4.097	6.974	8.941
70	1.743	4.116	6.982	8.921
75	1.754	4.137	6.992	8.900
80	1.765	4.159	7.004	8.885
85	1.778	4.183	7.018	8.867
90	1.792	4.210	7.034	8.850
95	-	-	-	-

Update

The values of the individual buffers with the corresponding temperatures are kept as up to date as possible.

However, they may be changed by the respective manufacturers.

5.12.10 Creating a Conductivity table

The templates for conductivity standards created according to these instructions are later used with the **CAL COND** command for the determination of the cell constant c of a conductivity measuring cell.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Defining a new conductivity standard

- Click on to open the **Inventory** window in **Equipment ► Solutions**.

- Add a conductivity standard with drag and drop to the solution list.

2 Adjusting the name and the expiry date of the conductivity standard

- Click on to open the **Properties** window.
- Enter the desired name in **Properties** ▶ **General** in the **Name** field.
  Define the expiry date of the conductivity standard in the **Expiry date** field under **Properties** ▶ **Specific data**.

3 Creating a conductivity table

- In **Properties** ▶ **Conductivity table**, click on to add new rows to the conductivity table.
- Define the entries in the **Temperature** and **Conductivity κ** columns in the conductivity table.

The conductivity values of the conductivity standards of Metrohm AG are indicated on the packaging.

Click on to delete a row from the conductivity table.

4 Saving a conductivity table

- Save the conductivity standard by clicking on .

The conductivity standard is saved. The name and the expiry date of the conductivity standard are automatically updated in the solution list.

Conductivity tables can be adjusted at any time. Adjustments do not have an effect on determinations that have already been carried out or on cell constants of a conductivity measuring cell that have already been determined.

See also

CAL COND – Properties (chapter 5.11.8.34, page 695)

5.12.11 Standards – Subsection

The following functions are available in **Equipment** ▶ **Standards**:

-
  Use **Import standards** to import data of a standard from an OSTD file (**O**MNIS **St**andar**d**).

-
  Use **Save** to save all changes.
-
  The standard is deleted with **Remove standard**. If the standard was used in a method, then a standard with the same name must be created again or another valid standard must be selected in the command parameters.

Definition

The term **Standards** is used in the OMNIS Software for:

- **NIR reflection standards** for reference standardization and for testing the signal noise.
- **NIR transmission standards** for reference standardization.

Commands

For instruments of the **2060 The NIR** type, the **ND Standard Reflection (R99) 2060 The NIR** standard can be used with commands of the **REF STD**, **VAL REF STD**, and **TEST NOISE** types. The standard must be held in front of the measuring probe during reference standardization, validation, or the test.

For instruments of the **OMNIS NIR Analyzer Liquid**, **OMNIS NIR Analyzer Liquid/Solid**, and **OMNIS NIR Analyzer Solid** types, standards can be used with a command of the **TEST NOISE** type.

With these instruments, you can choose between the **Reflection** and **Transmission** measuring modes in the commands. NIR reflection standards are required for the reference standardization, the validation, and the testing of the signal noise in **reflection mode**. NIR transmission standards are required for the **Transmission mode**.

In order to use a standard in the OMNIS Software, the standard must first be imported: *(see "Importing standards", chapter 5.12.11.2, page 1053)*.

Additional information on the commands: *(see "REF STD – Properties", chapter 5.11.8.19, page 621)*, *(see "VAL REF STD – Properties", chapter 5.11.8.18, page 618)*, *(see "TEST NOISE – Properties", chapter 5.11.8.22, page 628)*,

Overview list

The following information is displayed in the overview list of the standards:

Product type	English designation of the standard.
Name	Name of the standard. The name can be adjusted in the properties of the standard.

Serial number	Serial number of the standard.
Certification date	Date on which the standard was last certified. The standard can be re-certified via the regional Metrohm representative.

See also

Importing standards (chapter 5.12.11.2, page 1053)

REF STD – Properties (chapter 5.11.8.19, page 621)

Standards – Properties (chapter 5.12.11.1, page 1052)

TEST NOISE – Properties (chapter 5.11.8.22, page 628)

VAL REF STD – Properties (chapter 5.11.8.18, page 618)

5.12.11.1 Standards – Properties

After selecting the **Standards** functional unit, clicking on opens the **Properties** window.

The product information is displayed in the **General** subsection: *(see "Instruments – Properties", chapter 5.12.2.5, page 865)*. The following functions and information are available in the **Specific data** subsection, depending on the element selected:

Standard

Name	Enter the name of the standard.
Product type	Show the English designation of the standard.
Article number	Display the number that unambiguously identifies the standard.
Serial number	Display the serial number of the standard.
Certification date	Date on which the last certification was carried out.

See also

Importing standards (chapter 5.12.11.2, page 1053)

REF STD – Properties (chapter 5.11.8.19, page 621)

Standards – Subsection (chapter 5.12.11, page 1050)

VAL REF STD – Properties (chapter 5.11.8.18, page 618)

5.12.11.2 Importing standards

Prerequisite:

- At least one OMNIS standard file (***.ostd**) is available.
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting standards

- Click on to open the **Import standard** window in **Equipment ► Standards**.

2 Browsing for folder

- Select the folder in which the desired standard is saved.

3 Selecting the file

- Select the OMNIS standard file or enter the name of the OMNIS standard file in the **File name** field.

4 Confirming and importing the selection

- Click **[Open]** to confirm the selection.

The standard is imported into the OMNIS Software and is available in the command parameters of the **REF STD** command and the **VAL REF STD** command.

If the standard to be imported is already available, the standard and the certification date are overwritten with **[Update]**. The name of the standard is not modified.

If you delete a standard, it is permanently deleted from the database. The standard can no longer be used in the methods and the methods can no longer be executed. A different valid standard must be selected in the command parameters or a new standard must be imported.

See also

REF STD – Properties (chapter 5.11.8.19, page 621)

Standards – Properties (chapter 5.12.11.1, page 1052)

Standards – Subsection (chapter 5.12.11, page 1050)

VAL REF STD – Properties (chapter 5.11.8.18, page 618)

5.13 Models – Actions

You can execute the following actions in the subsections of the **Models** work area:

-

  In **Models** ▶ **Quantification models**, quantification models are developed, evaluated and published. Published quantification models can be used in the determination and reevaluation of predictions.

-

  In **Models** ▶ **Slope/y-intercept corrections**, Slope/y-intercept corrections are created, calculated and published for quantification models. Published slope/y-intercept corrections can be used in the determination and reevaluation of predictions.

-

  In **Models** ▶ **Identification models**, identification model are developed, evaluated and published. Published identification models can be used in the determination and reevaluation of predictions.

-

  In **Models** ▶ **Model hierarchies**, model hierarchies are edited, validated and published. Published model hierarchies can be used in the determination of predictions.

See also

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Creating identification model (chapter 5.13.3.4, page 1139)

Creating quantification model (chapter 5.13.1.7, page 1074)

Editing identification model (chapter 5.13.3.5, page 1141)

Editing quantification model (chapter 5.13.1.12, page 1082)

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

Publishing models (chapter 5.13.1.11, page 1080)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

Slope/y-intercept correction – Definition (chapter 5.13.2.6, page 1124)

Slope/y-intercept correction – Tab (chapter 5.13.2.7, page 1126)

5.13.1 Quantification models – Subsection

The following functions are available in **Models** ▶ **Quantification models**:

-

  Use **Create quantification model** to create a new quantification model. Quantification models can be developed, evaluated and published for use in the determination.

-

  Use **Import quantification model** to import an OPMO file (**O**MNIS **P**rediction **Mo**del) as a quantification model. Imported quantification models can be edited and used, depending on their types.

-

  Export quantification model exports the selected quantification models as OPMO files (**O**MNIS **P**rediction **Mo**del).

-

  Reports for the selected quantification models are generated with **Generate report**. The reports can be saved as a PDF file or also printed out.

-

  Duplicate quantification model duplicates the selected quantification models under the same name and with a consecutive number.

-

  Use **Properties** to open the properties of the selected quantification model.

-

  Delete quantification models deletes the selected quantification models and all quantification models published from them. Samples and subsamples contained in the quantification models are retained in the database.

Quantification models can be filtered by names and tags. Additional information on filtering quantification methods: *(see "Filtering tags", chapter 5.9.2, page 206)*

Overview list

The following information is displayed in the overview list:

Name	Name of the quantification model.
Version	Current version number of the quantification model. A new version is created automatically with each saving process.

Type	Type of the quantification model: ▪ **full** ▪ **light**
Last published version	Name and version number of the last published quantification model. Pre-calibration is also indicated with the icon.
Saved	Time at which the quantification model was last saved.
Tags	Existing tags assigned to the quantification model. Tags can be created only for the **Quantification model type full**.

If a Quantification model type light is imported into the OMNIS Software for which there is no Quantification model type full in the overview list, then **light** is displayed in the **Type** column.

The area that the model overview displays is on the right. This area shows information on the selected quantification models and thus enables a quick comparison of the models.

Additional information on the model overview: *(see "Model overview – Area", chapter 5.13.1.3, page 1063)*

See also

Creating and editing tags (chapter 5.9.1, page 203)

Creating quantification model (chapter 5.13.1.7, page 1074)

Exporting a model (chapter 5.13.1.9, page 1079)

Importing models (chapter 5.13.1.8, page 1077)

Model overview – Area (chapter 5.13.1.3, page 1063)

Models – Definition (chapter 5.13.1.1, page 1056)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Pre-calibration – Definition (chapter 5.13.1.13, page 1093)

5.13.1.1 Models – Definition

A **model** enables a sample to be analyzed on the basis of the measured spectrum.

A distinction is made between the following types of models:

- A **Quantification model** describes the dependence of a quantitative parameter of interest on the measured spectra of the samples.
  A quantification model enables the prediction of an analysis parameter for an unknown sample (e.g. water content 5.1%).
- A **Identification model** subdivides samples into different products (e.g. fructose, glucose, and lactose) based on the measured spectra.
  An identification model makes it possible to predict the identity of an unknown sample (e.g. fructose).
  A **Product** stands for a specific chemical substance or for a specific chemical substance with specific physical properties (e.g. particle size).
- A **Model hierarchy** can be used to structure **Identification models** and **Quantification models** hierarchically. Depending on the result of a prediction, further predictions will follow. Quantification models can also be provided with a **Slope/y-intercept correction**.
- **Identification models** and **Model hierarchies** can also be used for verification. During verification, the identity of an individual product is checked on the basis of a user input (e.g. fructose yes/no).

Models are created and managed in **Models** ▶ **Quantification models** or **Models** ▶ **Identification models**. Published models can be referenced in model hierarchies or directly in the **PREDICT** commands to evaluate spectra.

Published **Models** and **Slope/y-intercept corrections** can also be referenced in **Model hierarchies**.

To reevaluate quantitative results, published prediction models can be selected under **Samples** ▶ **Sample lists** ▶ **Results** ▶ **Predictions**.

Additional information on creating a quantification model: *(see "Creating quantification model", chapter 5.13.1.7, page 1074)*
Additional information on creating an identification model: *(see "Creating identification model", chapter 5.13.3.4, page 1139)*
Additional information on reprocessing predictions: *(see "Reprocessing predictions", chapter 5.10.13.5.1, page 363)*

Type full and type light

Each model can be available as **Type full** or as **Type light**, e.g. **Quantification model type full** and **Quantification model type light**:

- **Type full** model
  A type full model contains all the information necessary to create, optimize and validate the model. The type full model can be edited and saved. When publishing a model, the OMNIS Software creates a type light model.

- **Type light** model
  A type light model contains only the data for calculating the parameter of interest. In addition, the data preprocessing and wavelength ranges used can be viewed. *(see "Reprocessing predictions", chapter 5.10.13.5.1, page 363)*, *(see "PREDICT – Parameters", chapter 5.11.8.16, page 610)*

If a type light model is imported into the OMNIS Software for which there is no type full model in the overview list, then the model will be displayed in the **Type** column as **light**.

See also

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Creating identification model (chapter 5.13.3.4, page 1139)

Creating quantification model (chapter 5.13.1.7, page 1074)

Data preprocessing – Area (chapter 5.13.1.17, page 1100)

Editing identification model (chapter 5.13.3.5, page 1141)

Editing quantification model (chapter 5.13.1.12, page 1082)

Figures of merit – Definition (chapter 5.13.1.19, page 1103)

Histogram – Area (chapter 5.13.1.15, page 1098)

Identification model – Tab (chapter 5.13.3.1, page 1129)

Influence plot – Area (chapter 5.13.1.21, page 1112)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

Report template – Directory (chapter 5.10.1.4.1, page 233)

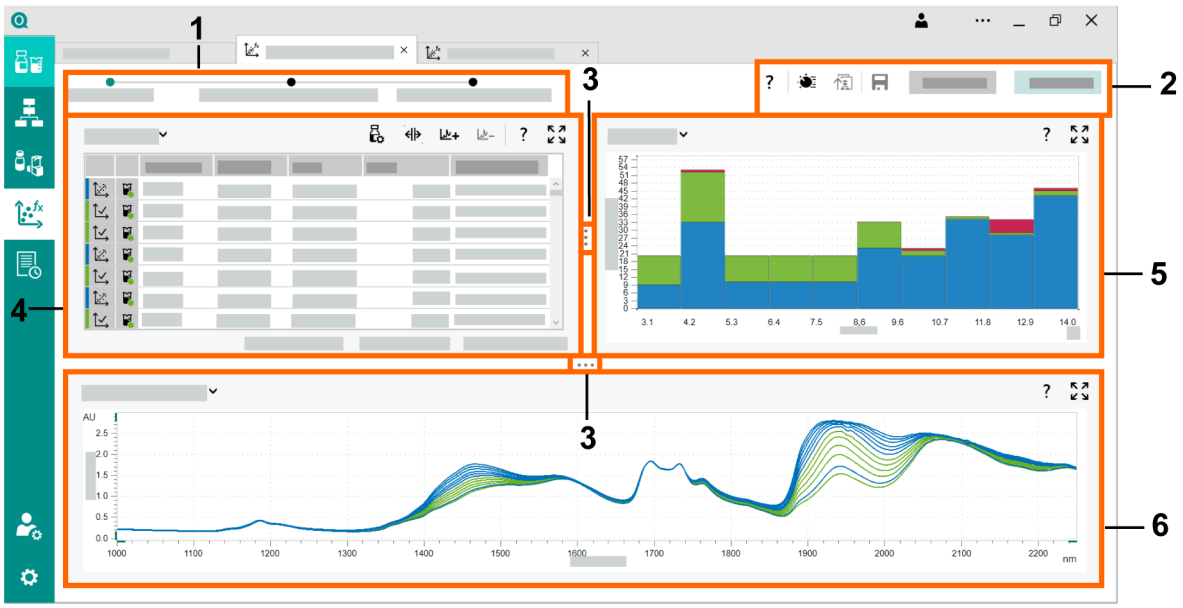
Spectra list – Area (chapter 5.13.1.14, page 1094)

Spectra overlay – Area (chapter 5.13.1.16, page 1099)

Wavelength range – Area (chapter 5.13.1.18, page 1102)

5.13.1.2 Quantification model – Tab

"Select samples" process step



1 Navigator
Selection from the **Select samples**, **Parameterize quantification model** and **Validate quantification model** process steps.

If incorrect entries have been made in the individual areas, then the respective process steps are displayed in **red**. By default, the process steps are displayed in **black** and the current selection in **green**.

2 Toolbar
Calculate, save and publish the quantification model.

Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

3 Divider
The size of the individual areas can be adjusted with the divider.

4 Spectra list
Displays spectra that are used in the quantification model. See detailed image *Spectra list*.

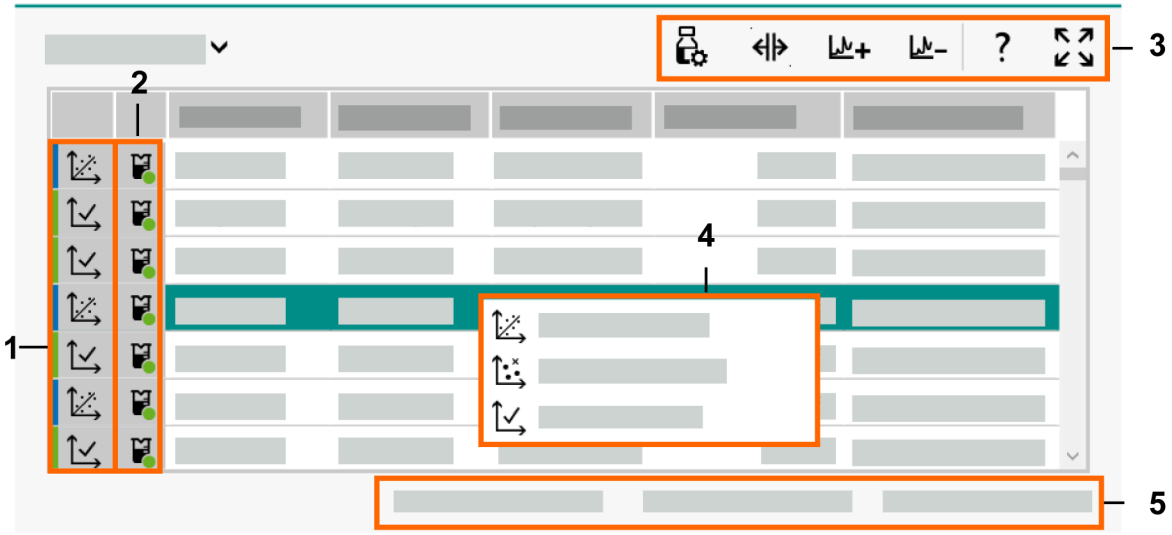
Selecting a spectrum in the list also causes that spectrum to be highlighted in the spectra overlay, in the correlation plot, and in the influence plot.

5 Histogram
Shows the frequency distribution of datasets of the reference parameter. *(see "Histogram – Area", chapter 5.13.1.15, page 1098)*

6 Spectra overlay
Shows the raw spectra from the spectra list overlaid. *(see "Spectra overlay – Area", chapter 5.13.1.16, page 1099)*

Selecting a spectrum in the Spectra list also causes that spectrum to be highlighted in the spectra list, in the correlation plot, and in the influence plot.

Spectra list



1	**Dataset display** Shows the dataset to which the spectrum belongs.	**2**	**Availability of the subsample in the database** Shows if the subsample is available in the database or if the spectrum has been imported from an external file.
3	**Toolbar** Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*	**4**	**Context menu** With the context menu, a spectrum can be assigned to a dataset.
5	**Number of spectra per dataset** Shows the number of spectra in the individual datasets.		

"Parameterize quantification model" process step

The **Spectra overlay**, **Wavelength range**, **Data preprocessing**, and **Loading plot** can be displayed in any area marked in orange:

- **Spectra overlay**
  Shows the preprocessed spectra from the spectra list overlaid. *(see "Spectra overlay – Area", chapter 5.13.1.16, page 1099)*

  Clicking on the **Optimize parameterization** button calculates or optimizes data preprocessings and wavelength ranges.

- **Wavelength range**
  The desired wavelength range of the spectra overlay can be selected. *(see "Wavelength range – Area", chapter 5.13.1.18, page 1102)*

- **Data preprocessing**
  The desired procedures for the data preprocessing of spectra can be selected and their order can be determined. *(see "Data preprocessing – Area", chapter 5.13.1.17, page 1100)*

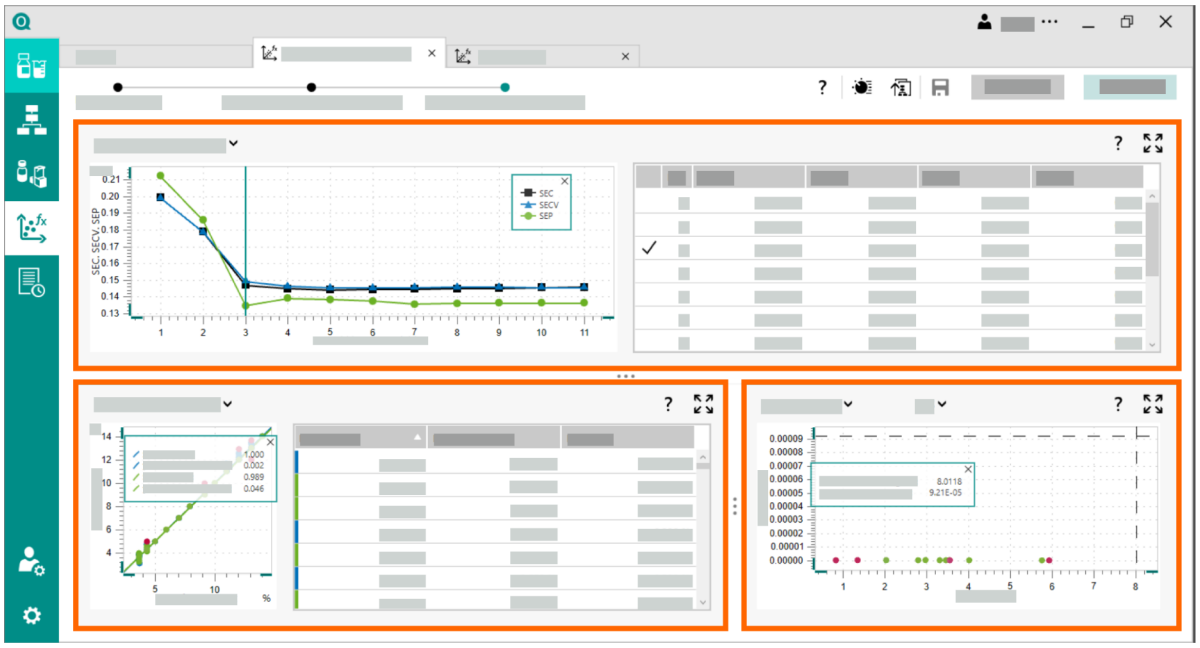
- **Loading plot**
  Shows the intensity of the loadings for each latent variable as a chart.

  Clicking on the **Optimize parameterization** button calculates or optimizes data preprocessings and wavelength ranges.

  (see "Loading plot – Area", chapter 5.13.1.22, page 1113)

"Validate quantification model" process step

The **Figures of merit**, **Influence plot**, **Correlation plot**, **Loading plot**, and **Score plot** can be displayed in any area marked in orange:



- **Figures of merit**
  Shows the figures of merit for the number of latent variables. The values are displayed as a chart and as a table. *(see "Figures of merit – Definition", chapter 5.13.1.19, page 1103)*

- **Correlation plot**
  Shows the correlation of the measured quantities **Reference value** and **Calculated value**. The values are displayed as a chart and as a table. The assignment to the calibration dataset or validation dataset is shown in color.*(see "Correlation plot – Area", chapter 5.13.1.20, page 1108)*

- **Score plot**
  Shows the scores of the spectra using the PLS calculation method as a chart. The latent variables for the **x-axis** and **y-axis** are selected. *(see "Score plot – Area", chapter 5.13.1.23, page 1114)*

- **Influence plot**
  The distribution of the datasets as a value pair of **Hotelling's T²** and **Q residuals** is displayed as a chart. **PLS** and **PCA** are available as calculation methods. *(see "Influence plot – Area", chapter 5.13.1.21, page 1112)*

- **Loading plot**
  Shows the intensity of the loadings for each latent variable as a chart.*(see "Loading plot – Area", chapter 5.13.1.22, page 1113)*

See also

Copying table (chapter 5.2.8, page 172)

Creating quantification model (chapter 5.13.1.7, page 1074)

Editing quantification model (chapter 5.13.1.12, page 1082)

Models – Definition (chapter 5.13.1.1, page 1056)

5.13.1.3 Model overview – Area

The area for the model overview is displayed on the right side under **Models** ▶ **Quantification models**. Model overview allows a quick comparison of the selected quantification models, based on the information shown. Only the first 5 selected quantification models are displayed in the Model overview.

The following information is available on the selected quantification models in the Model overview:

Some of the information listed is not displayed for pre-calibration.

Quantification model	
Version number (saved)	The last saved version of the quantification model. A new version of the model saved is created automatically each time a quantification model is saved.
Version number (published)	The last published version of the quantification model or of the pre-calibration. The published quantification model uses the version of the model saved last.
Version number (saved and published)	The last saved and published version of the quantification model or of the pre-calibration. **(saved and published)** appears if the saved model has not been changed and saved after publishing the quantification model.
SEC	Standard error of calibration.
SECV	Standard error of cross-validation.
SEP	Standard error of prediction.
R^2CV	Coefficient of determination of cross-validation.
R^2P	Coefficient of determination of prediction.
Number of latent variables	Number of selected latent variables.

Additional information on figures of merit: *(see "Figures of merit – Definition", chapter 5.13.1.19, page 1103)*

Datasets	
Calibration dataset	The number of spectra that are assigned to the calibration dataset.

Datasets	
Validation dataset	The number of spectra that are assigned to the validation dataset.
Outlier dataset	The number of spectra that are assigned to the outlier dataset.

Data preprocessings

Detrend	
Start wavelength	Lower limit of the wavelength range.
End wavelength	Upper limit of the wavelength range.

Gap-Segment	
Derivative order	Specification as to how often the spectrum is to be derived.
Segment size	Segment size.
Gap size	Distance between the two segments.

Savitzky-Golay	
Derivative order	Specification as to how often the spectrum is to be derived.
Filter width	Filter width.
Polynomial degree	Degree of the polynomial function.

SNV	
Start wavelength	Lower limit of the wavelength range.
End wavelength	Upper limit of the wavelength range.

Additional information on data preprocessing: *(see "Data preprocessing – Area", chapter 5.13.1.17, page 1100)*

No data preprocessing can be displayed for pre-calibrations.

Wavelength ranges	
from–to	Start wavelength and End wavelength.

Additional information on wavelength ranges: *(see "Wavelength range – Area", chapter 5.13.1.18, page 1102)*
No wavelength ranges can be displayed for pre-calibrations.

Correlation plot

Additional information on the Correlation plot: *(see "Correlation plot – Area", chapter 5.13.1.20, page 1108)*
No correlation plot can be displayed for pre-calibrations.

See also

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Creating quantification model (chapter 5.13.1.7, page 1074)

Data preprocessing – Area (chapter 5.13.1.17, page 1100)

Editing quantification model (chapter 5.13.1.12, page 1082)

Figures of merit – Area (chapter 5.13.1.19.1, page 1106)

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

Pre-calibration – Definition (chapter 5.13.1.13, page 1093)

Publishing models (chapter 5.13.1.11, page 1080)

Wavelength range – Area (chapter 5.13.1.18, page 1102)

5.13.1.4 Quantification model – Properties

Clicking on under **Models** ▶ **Quantification models** opens the **Properties** window. The following information on the selected quantification model is available in the **General** subsection:

General

Quantification model	
Name	Name of the quantification model.
Object ID	Identification number of the quantification model.
Version	Version number of the quantification model. A new version is created automatically each time a quantification model is saved.
Created	Time at which the quantification model was created.
Created by	User ID of the user that created the quantification model.

Saved	Time at which the quantification model was last changed.
Saved by	User ID of the user that changed the quantification model.
Last published version	
Name	Name of the last published version of the quantification model.
Object ID	Identification number of the last published version of the quantification model.
Saved	Time at which the last published version of the quantification model was saved.
Saved by	User ID of the user that last published the quantification model.

Open the **Properties** window by clicking on under **Models** ▶ **Quantification models** within an opened quantification model. In the 2 subsections **General** and **Parameters**, the following functions and information are available:

General

Name	Name of the quantification model (can be edited, max. 255 characters).
Object ID	Identification number of the quantification model.
Version	Version number of the quantification model. A new version is created automatically each time a quantification model is saved.
Created	Time at which the quantification model was created.
Created by	User ID of the user that created the quantification model.
Saved	Time at which the quantification model was last changed.
Saved by	User ID of the user that changed the quantification model.

Parameters

Cross-validation	

Cross-validation method

The cross-validation method validates the quantification model. Spectra are obtained from the calibration dataset. A quantification model is created on the basis of this reduced dataset and applied to the previously obtained spectra. This process is repeated as often as needed until all of the spectra of the data set have been removed once.

The values of the spectra are displayed after the calculation of the quantification model in **Correlation plot**. *(see "Correlation plot – Area", chapter 5.13.1.20, page 1108)*

Selecting the desired cross-validation method:

- **Leave-One-Out** (default value):
  The Leave-One-Out procedure validates the quantification model. A spectrum is obtained from the calibration dataset. A quantification model is created on the basis of this reduced dataset and applied to the previously obtained spectrum. This process is repeated as often as needed until all of the spectra of the data set have been removed once.

Notice: For spectra lists with more than 70 spectra, the **Leave-One-Out** procedure may take a very long time.

- **K-fold**:
  The procedure splits the calibration dataset into blocks of equal size. A block is subsequently taken from this dataset. A model is created on the basis of this reduced dataset and applied to the previously obtained block. This process is repeated as often as needed until all of the blocks of the dataset have been removed once.
  If **K-fold** is selected, then the **Number of blocks** parameter also appears. The parameters define the number *k* of blocks in the model and must be smaller than the number of spectra.
  Select the desired algorithm:
  - **Random**:
    At each iteration, the algorithm splits the spectra of the calibration dataset into randomly chosen but equal-size blocks.
  - **Fixed Blocks (DUPLEX)**:
    The algorithm splits the spectra into non-random, equal-size blocks. The variance of the spectra in each block is maximized.

Notice: For very large spectra lists, the **K-fold** procedure is recommended.

Outlier limits

Significance level

Enter the desired significance level.

Additional information on the **Influence plot**: *(see "Influence plot – Area", chapter 5.13.1.21, page 1112)*

See also

Audit Trail – Directory (chapter 5.14.5, page 1177)

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Creating quantification model (chapter 5.13.1.7, page 1074)

Editing quantification model (chapter 5.13.1.12, page 1082)

Influence plot – Area (chapter 5.13.1.21, page 1112)

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

Publishing models (chapter 5.13.1.11, page 1080)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

5.13.1.5 Reprocessing a quantification model

If reference values of the samples that the quantification model are based on need to be edited during processing, then they can be changed directly in the sample list.

Reprocessing samples

Prerequisite:

- The samples are used in a quantification model.
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Opening a sample list

- Open the sample list with the samples that the quantification model is based on in **Samples** ▶ **Sample lists**.

2 Changing a reference value

- Change the required reference value of the sample in question.
  This is only possible:
  if the field was marked **editable** when creating the sample profile.
  or
  if a **CALC** command was used for the calculation of the reference value. Then make the required settings in **Results** ▶ **Calculations** by clicking on fx=.
- Save the sample list by clicking on .

3 Updating a quantification model

- Open the required quantification model in question in **Models** ▶ **Quantification models**.

The message **Reference values of quantification model were changed** appears.

4 Recalculating and republishing the quantification model

- Click on **[Calculate]** to recalculate the quantification model. Check the data in the **Validate quantification model** process step and adjust it if necessary. *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*
- Save the quantification model by clicking on and then re-publish it, if necessary. *(see "Nearest Neighbor Distance – Definition", chapter 5.13.1.10, page 1080), (see "Publishing models", chapter 5.13.1.11, page 1080)(see "Publishing models", chapter 5.13.1.11, page 1080)*

See also

Audit Trail – Directory (chapter 5.14.5, page 1177)

CALC – Parameters (chapter 5.11.8.64, page 768)

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Creating quantification model (chapter 5.13.1.7, page 1074)

Editing sample list (chapter 5.10.1.2, page 212)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

Publishing models (chapter 5.13.1.11, page 1080)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.1.6 Preparing quantification model

These instructions describe 3 options how reference values can be entered before, during or after the measurement of the samples.

Alternatively, samples with already defined reference values can be imported from the XDS instrument or the DS instrument into the quantification model. Additional information on importing spectra and their reference parameters: *(see "Importing spectra and reference parameters", chapter 5.13.1.14.1, page 1098)*

- *Entering known reference values manually*
- *Entering reference values with the REQUEST command*
- *Entering reference values with the CALC command*

Entering known reference values manually

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Creating operating procedure with method

- Create a new method in **Processes** ▶ **Methods**.
- Click on to insert a **MEAS SPEC** command in the method. Parameterize the command in such a way that it acquires spectra of the samples. *(see "MEAS SPEC – Properties", chapter 5.11.8.31, page 674)*
- Assign the method to an operating procedure.

2 Creating sample profile

- In **Samples** ▶ **Sample profiles**, click on .
- Enter the desired name in the **Name of the sample profile** field.

3 Defining reference parameters

- Add as many input fields as there are reference parameters in the **Sample data** area by clicking on . The number of reference parameters yields the number of different quantification models that can be created with the sample.
- Enter the name of the reference parameter in the **Field name short** field.
- Select the **Number** option in the **Type of input field** field.
- Select the **Input field** option in the **Use as** field.
- Enable the **Editable field** check box so that the reference values can be entered.
- Enable the **Allow empty field** check box so that the **Default value** field can be left empty.
- Enable the **Force entry** check box so that the entry of a value is to forced for empty fields before the determination is started.
- In the **Operating procedures / subsamples** area, select the created operating procedure and enter the number "1" in **Number of subsamples**.
- Save the sample profile by clicking on .

4 Editing sample list

- In **Samples** ▶ **Sample lists**, create a new sample list or open an existing sample list.

- Select the sample profile and add the required number of samples to the sample list by clicking on .
- Enter the default reference values of the available reference samples under the reference parameters.
- Save the sample list by clicking on .
- Carry out the determination of the subsamples.

Entering reference values with the REQUEST command

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Creating sample profile

- In **Samples** ▶ **Sample profiles**, click on .
- Enter the desired name in the **Name of the sample profile** field.

2 Defining reference parameters

- Add as many input fields as there are reference parameters in the **Sample data** area by clicking on . The number of reference parameters yields the number of different quantification models that can be created with the sample.
- Enter the name of the reference parameter in the **Field name short** field.
- Select the **Number** option in the **Type of input field** field.
- Select the **Input field** or **Result** option in the **Use as** field.
  If the **Input field** option was selected, then enable the following check boxes:
  - Enable the **Editable field** check box so that the reference values can be entered.
  - Enable the **Allow empty field** check box so that the **Default value** field can be left empty.
- Save the sample profile by clicking on .

3 Creating operating procedure with method

- Create a new method in **Processes** ▶ **Methods**.

- Click on to insert a **REQUEST** command in the method. Parameterize the command in such a way that it writes to the sample data. *(see "REQUEST – Parameters", chapter 5.11.8.77, page 794)*
- Click on to insert a **MEAS SPEC** command in the method. Parameterize the command in such a way that it acquires spectra of the samples. *(see "MEAS SPEC – Properties", chapter 5.11.8.31, page 674)*
- Assign the method to an operating procedure.

4 Assigning operating procedures to the sample profile

- Open the created sample profile in **Samples** ▶ **Sample profiles**.
- In the **Operating procedures / subsamples** area, select the created operating procedure.
- Under **Number of subsamples**, enter the number "1".

5 Entering reference values

- In **Samples** ▶ **Sample lists**, create a new sample list or open an existing sample list.
- Select the sample profile and add the required number of samples to the sample list by clicking on .
- Save the sample list by clicking on .
- Carry out the determination of the subsamples.
- During the determination of the sample, enter the reference values in the corresponding fields in an opened sample list in **Curves and data** ▶ **Live data**.

Entering the reference values from the primary processes with the CALC command

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- Use the **MEAS SPEC** command in addition to a primary procedure that determines the reference values (e.g. of a titration). Ideally, split the procedures over more than one subsample.

1 Creating sample profile

- In **Samples** ▶ **Sample profiles**, click on .

- Enter the desired name in the **Name of the sample profile** field.

2 Defining reference parameters

- Add as many input fields as there are reference parameters in the **Sample data** area by clicking on . The number of reference parameters yields the number of different quantification models that can be created with the sample.
- Enter the name of the reference parameter in the **Field name short** field.
- Select the **Number** option in the **Type of input field** field.
- Select the **Result** option in the **Use as** field.
- Save the sample profile by clicking on .

3 Extending the method for the primary procedure with a CALC command

- Open the method for the primary procedure in **Processes** ▶ **Methods**.

  Click on to insert a **CALC** command in the method. Parameterize the command in such a way that it writes the result of the primary method in the reference parameter. *(see "CALC – Parameters", chapter 5.11.8.64, page 768)*
- Assign the method to an operating procedure.

4 Creating operating procedure with method

- Create a new method in **Processes** ▶ **Methods**.
- Click on to insert a **MEAS SPEC** command in the method. Parameterize the command in such a way that it acquires spectra of the samples. *(see "MEAS SPEC – Properties", chapter 5.11.8.31, page 674)*
- Assign the method to an operating procedure.

5 Assigning operating procedures to the sample profile

- Open the created sample profile in **Samples** ▶ **Sample profiles**.
- Select the previously created operating procedures of the primary procedure and the spectroscopic analysis in the **Operating procedures / subsamples** area.
- Under **Number of subsamples**, enter the number "1" in each case.

6 Transferring reference values

- In **Samples** ▶ **Sample lists**, create a new sample list or open an existing sample list.
- Select the sample profile and add the required number of samples to the sample list by clicking on .
- Save the sample list by clicking on .
- Carry out the determination of the subsamples.

During the determination, the values that were determined by the primary procedure are written in the reference parameters.

See also

CALC – Parameters (chapter 5.11.8.64, page 768)

Creating and deleting sample lists (chapter 5.10.1.1, page 211)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Creating quantification model (chapter 5.13.1.7, page 1074)

Importing spectra and reference parameters (chapter 5.13.1.14.1, page 1098)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

REQUEST – Parameters (chapter 5.11.8.77, page 794)

Starting determination (chapter 5.10.8.6, page 304)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.1.7 Creating quantification model

Metrohm also offers ready-to-use quantification models for specific applications. These models are called pre-calibrations and can be purchased. Additional information on the pre-calibrations: *(see "Pre-calibration – Definition", chapter 5.13.1.13, page 1093)*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses and function licenses are enabled.
  Additional information: *Metrohm Knowledge Base*

1 Creating new quantification model

- In **Models** ▶ **Quantification models** click on .

2 Entering name

- Enter the desired name in the **Name of the quantification model** field.

The name can be changed at any time in the opened quantification model in **Properties** ▶ **General**.

3 Selecting spectra and reference parameters

- Add the spectra either from the Sample lists or the Search queries of the OMNIS Software or import them from an XDS instrument or a DS instrument.

  Add spectra from sample lists or search queries of the OMNIS Software

  – Display all the sample lists saved in the database by clicking on **Sample lists**.
    or
  – Display all the search queries saved in the database by clicking on **Search queries**.
  – Select sample lists or search queries from which spectra are added to the quantification model.
  – The table on the right shows all Reference parameter and their units in the selected sample lists or search queries. Select the desired reference parameter from this table.
    Note: If the required reference parameter has several designations in the sample lists or search queries, all these designations can be selected.
  – Click on **[Continue]** to confirm the selection.

  or

  Importing spectra from XDS or DS instruments

  – To import spectra that were acquired with an XDS or DS instrument, click on **XDS/DS import**.
  – Click on .
  – Select the spectra file (.da) that is to be imported.
  – Click **[Open]** to confirm the selection.
  – Click on **[Continue]**.

No more than 1,000 spectra should be added to the quantification model because such a high number of spectra can lead to an impairment of the software performance.

4 Setting reference parameter

- Enter the name of the quantification model in the **Name of the quantification model** field, if required.
- The table shows all reference parameters and their units in the previously selected sample lists, search queries or DA files. In addition, the selection of reference parameters from the previous step is retained for sample lists and search queries.
  If required, adjust the selection of reference parameters in the table.

If the required reference parameter has several designations in the sample lists or search queries, then all these designations can be selected.

- Enter the desired name used in the quantification model in the **Name of reference parameter** input field.
- Select the **Unit of reference parameter** to be used in the quantification model.
- Enter the desired number of **Decimal places** that will be displayed in the results of the quantification model.

All spectra that have the selected designations of the reference parameter are added to the quantification model.

5 Developing or manually editing a quantification model with OMNIS Model Developer

Develop the quantification model automatically with the OMNIS Model Developer (OMD) or edit it manually.

- **Developing the quantification model with OMD**
  - Develop the new quantification model with the OMD by clicking on **[Start OMD]**. Instructions for developing the quantification model with the OMD: *(see "Developing quantification models with OMNIS Model Developer (OMD)", chapter 5.13.1.24, page 1114)*

or

- **Creating and manually editing the quantification model**
  - Create the new quantification model by clicking on **[Create]**.
  - Save the quantification model by clicking on .
  - Edit the quantification model, i.e. go through the process steps of the navigator and adjust the data as required. Instructions for editing quantification models: *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*

See also

Copying table (chapter 5.2.8, page 172)

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Developing quantification models with OMNIS Model Developer (OMD) (chapter 5.13.1.24, page 1114)

Editing quantification model (chapter 5.13.1.12, page 1082)

Importing spectra and reference parameters (chapter 5.13.1.14.1, page 1098)

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

Pre-calibration – Definition (chapter 5.13.1.13, page 1093)

Preparing quantification model (chapter 5.13.1.6, page 1069)

Publishing models (chapter 5.13.1.11, page 1080)

Reprocessing a quantification model (chapter 5.13.1.5, page 1068)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.1.8 Importing models

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- At least one OMNIS model file (**.opmo**) is available.

- If pre-calibrations are imported into the OMNIS Software, then the corresponding function license should also be available and activated for their use. Instructions for activating the function license: *(see "Activating the function license", chapter 4.2.3, page 35)*.

1 Selecting model

- Select a corresponding model in the following subsections:
  - **Models ▶ Quantification models**
  - **Models ▶ Identification models**
- Click on to open the window for importing the model.

2 Browsing for folder

- Select the folder in which the required model is saved.

3 Selecting file

- Select the OMNIS model file or enter the name of the OMNIS model file in the **File name** field.

4 Confirming and importing selection

- Click **[Open]** to confirm the selection.

The model is imported into the OMNIS Software. During a pre-calibration, the model is indicated with the icon.

If the model is already available in the database, then the model can either be overwritten or created as a new version.

See also

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Creating identification model (chapter 5.13.3.4, page 1139)

Creating quantification model (chapter 5.13.1.7, page 1074)

Exporting a model (chapter 5.13.1.9, page 1079)

Models – Definition (chapter 5.13.1.1, page 1056)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

Pre-calibration – Definition (chapter 5.13.1.13, page 1093)

5.13.1.9 Exporting a model

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- At least one model is available in the corresponding overview list.

1 Selecting models

- Select the corresponding models in the following subsections:
  - **Models ▶ Quantification models**
  - **Models ▶ Identification models**
- Open the window for exporting the models by clicking on .

2 Selecting the export type

- Select the **Export type** from the selection list.
  - **Type full**
  - **Type light**

Only models of the same type can be exported at the same time. Additional information on the export types **Type full** and **Type light**: *(see "Models – Definition", chapter 5.13.1.1, page 1056)*

3 Selecting or entering a target folder

- Select the target folder by clicking on or enter the absolute path in the address bar.

4 Creating OMNIS model files

- Export the OMNIS model files (OPMO files) into the target folder by clicking on **[Export]**. One or more OPMO files are exported under the respective name of the models.
- Click on **[Open target folder]** to open the target folder.

All time indications are converted into Coordinated Universal Time (UTC±00:00) when exporting. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.

The local time on the computer is used for the date and time displayed in the file name.

See also

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Creating identification model (chapter 5.13.3.4, page 1139)

Creating quantification model (chapter 5.13.1.7, page 1074)

Importing models (chapter 5.13.1.8, page 1077)

Models – Definition (chapter 5.13.1.1, page 1056)

Pre-calibration – Definition (chapter 5.13.1.13, page 1093)

5.13.1.10 Nearest Neighbor Distance – Definition

Nearest Neighbor Distance can be enabled for the publication of a quantification model.

The procedure selects the first spectrum from the calibration dataset and calculates the distances of all spectra from the calibration dataset to this selected spectrum. This process is repeated as often as needed until the minimum distances of all of the spectra of the dataset have been determined. This results in a **NND limit**. During routine analysis, this value is compared with the NND value of the unknown spectra. The NND value of the unknown spectra and the NND limit are each stored in a variable.

Additional information on the results of **Nearest Neighbor Distance**: *(see "PREDICT – Command variables", chapter 5.11.8.16.1, page 611)*

See also

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

Publishing models (chapter 5.13.1.11, page 1080)

5.13.1.11 Publishing models

To use a model for determinations and repredictions, the model must be published. This means that the model can still be developed further without impacting the published version – and the determinations and repredictions carried out with it.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

- The model to be published was calculated and saved.

1 Opening model

- Open the desired model in the following subsections:
  - **Models ▶ Quantification models**
  - **Models ▶ Identification models**

2 Opening the dialog

- Open the desired dialog by clicking on :
  - **Publish quantification model**
  - **Publish identification model**

3 Updating methods (optional)

- To update methods that use this model, enable the **Update methods** check box.

This option only applies if the existing and already used model was changed and is published once again. Signed and published methods will not be changed. If the filtering of the data permissions is enabled, then only methods with the data permissions of the currently logged-in user will be updated.

Additional information on the data permissions: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

4 Calculating the Nearest Neighbor Distance (optional)

This option is available only for quantification models. If this option is enabled, then the duration of the publication may increase.

Additional information on Nearest Neighbor Distance:

- Enable the Calculate **Nearest Neighbor Distance** check box to calculate the NND-limit and save the result in the published quantification model.

Additional information on the results of Nearest Neighbor Distance: *(see "PREDICT – Command variables", chapter 5.11.8.16.1, page 611)*

5 Publishing the model

- Publish the model by clicking on **[Publish]**.

The last published version of the model is displayed in the overview list and is available for the determination in the parameters of the

PREDICT command. Published quantification models can be used for the reevaluation of results.

Additional information on using models in determination or reevaluation:

- *(see "PREDICT – Parameters", chapter 5.11.8.16, page 610)*
- *(see "Reprocessing predictions", chapter 5.10.13.5.1, page 363)*

If a published model used in a method is deleted, then the method cannot be executed anymore.

See also

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Editing identification model (chapter 5.13.3.5, page 1141)

Editing quantification model (chapter 5.13.1.12, page 1082)

Exporting a model (chapter 5.13.1.9, page 1079)

Importing models (chapter 5.13.1.8, page 1077)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.1.12 Editing quantification model

These instructions describe how to manually edit the quantification model. With the help of the OMNIS Model Developer, it is possible to develop a quantification model automatically.
Additional information on the OMNIS Model Developer: *(see "Developing quantification models with OMNIS Model Developer (OMD)", chapter 5.13.1.24, page 1114)*

A quantification model is edited manually in 3 steps:

- *Select samples*
- *Parameterize quantification model*
- *Validate quantification model*

The following **prerequisites** must be fulfilled for all 3 steps:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The quantification model is created: *(see "Creating quantification model", chapter 5.13.1.7, page 1074)*

Selecting samples

Prerequisite:

- The **Models** ► **Quantification models** subsection is opened.
- A quantification model is open and at the front. The navigator is in the **Select samples** process step.

Additional information on the navigator: *(see "Quantification model – Tab", chapter 5.13.1.2, page 1059)*

1 Adding spectra (optional)

Selecting spectra and reference parameters

- Add spectra to the spectra list by clicking on .
  The current reference parameter of the quantification model is displayed in the **Reference parameter/unit of the quantification model** field.

- Add the spectra either from the Sample lists or the Search queries of the OMNIS Software or import them from an XDS instrument or a DS instrument.

  Add spectra from sample lists or search queries

  – Display all the sample lists saved in the database by clicking on **Sample lists**.
  or
  – Display all the search queries saved in the database by clicking on **Search queries**.
  – Select sample lists or search queries from which spectra are added to the quantification model.
  – The table on the right shows all Reference parameter and their units in the selected sample lists or search queries. Select the desired reference parameter from this table.
  Note: If the required reference parameter has several designations in the sample lists or search queries, all these designations can be selected.
  – Click on **[Add]** to add all spectra that have the selected reference parameters.

  or

  Importing spectra from XDS or DS instruments

  – To import spectra that were acquired with an XDS or DS instrument, click on **XDS/DS import**.
  – Click on .
  – Select the spectra file (.da) that is to be imported.
  – Click **[Open]** to confirm the selection.
  – Click on **[Continue]**.
  – The current reference parameter of the quantification model is displayed in the **Reference parameter/unit of the quantification model** field.
  Select the desired reference parameter from the table.
  – Click on **[Add]** to add all spectra that have the selected reference parameter.

- The reference parameters of the added spectra apply the name and unit of the current reference parameter in the quantification model.

No more than 1,000 spectra should be added to the quantification model because an excessively high number of spectra can lead to an impairment of the software performance.

2 Deleting spectra (optional)

- To delete spectra from the spectra list, select the spectra and click on .

Note: The spectra are then permanently deleted from the quantification model.

3 Editing reference parameters (optional)

- Click on .
  All available reference parameters of the spectra from the quantification model are displayed in the **Reference parameters/unit** list. The reference parameters of the spectra currently used in the quantification model are highlighted in the list.
- Select the required names of the reference parameter in the **Reference parameters/unit** list.

If the desired reference parameter has several designations, all of these designations can be selected in the list at the same time.

- Enter the desired name used in the quantification model in the **Name of reference parameter** input field.
- Select the **Unit of reference parameter** to be used in the quantification model.
- Enter the desired number of **Decimal places** that will be displayed in the results of the quantification model.
- Click on **[Apply]** to apply the selected reference parameter with the entered name, the unit, and the defined decimal places.

Spectra that do not have any of the selected reference parameters or that have an invalid reference parameter are highlighted in red and indicated with in the **Spectra list**. These spectra should be removed from the quantification model.

4 Editing the name und parameters of the quantification model (optional)

- Click on **Properties** ▶ **Parameters** to open the parameters of the quantification model.
- Click on **Properties** ▶ **Parameters** to open the parameters of the quantification model.
- Select **Cross-validation method** under **Cross-validation**:
  If **K-fold** was selected:
  - Enter **Number of blocks** into which the calibration dataset will be split.
  - Select **Splitting algorithm**:

  Random
  Fixed Blocks (DUPLEX)

- Define the significance level for outlier detection in the **Significance level** field under **Outlier limits**.

Additional information on the Influence plot: *(see "Influence plot – Area", chapter 5.13.1.21, page 1112)*
Additional information on the Correlation plot: *(see "Correlation plot – Area", chapter 5.13.1.20, page 1108)*

5 Splitting dataset automatically or manually

Splitting spectra list automatically

- In **Select samples** ▶ **Spectra list**, click on .
- Enable the toggle switch **Detect outliers** to automatically assign spectra to the outlier dataset and to define the significance level. Additional information on the significance level:
- Enable the **Determine validation dataset** toggle switch and define the percentage of spectra to be used for the validation dataset in the **Percentage** field.
- The following options can be enabled before the splitting of the dataset:
  - **Apply parameterization**: Applies the data preprocessings selected in the **Parameterize quantification model** process step and the defined wavelength ranges to the spectra before the dataset is determined.
  - **Keep outliers**: The already existing outliers are retained and not taken into account in the split. This option can lead to an increase in the size of the outlier dataset, even if the significance level is not changed.
  - **Keep validation dataset**: The existing validation dataset is retained and not taken into account in the split. This option leads to an increase in the size of the validation dataset, even if the percentage of the validation dataset is not changed.
- Click on **[Split]** to confirm.
- If necessary, manually reprocess the automatically split spectra list.

or

Splitting spectra list manually

- Right-click on one or more spectra to open the context menu and assign the spectrum to the **Calibration dataset**, **Outlier dataset** or **Validation dataset**.

At least 2 spectra must be assigned to the calibration dataset so that the quantification model can be calculated.

As soon as at least one spectrum is selected in the spectra list, the spectrum is highlighted in the **Spectra overlay** area.

In the **Histogram** and **Spectra overlay** areas, spectra in the calibration dataset are marked **blue**, spectra in the validation dataset are marked **green** and spectra in the outlier dataset are marked **red**.

In the **Spectra list** area, the assignments are represented by the following icons:

- spectrum is part of the calibration dataset.
- spectrum is part of the validation data set.
- spectrum is part of the outlier dataset.

Parameterizing the quantification model

Prerequisite:

- The **Models** ▶ **Quantification models** subsection is opened.
- A quantification model is open and at the front.
- All actions in the **Select samples** process step have been executed.

1 Change to the "Parameterize the quantification model" process step

- In the navigator, change to the next process step of editing the quantification model by clicking on **Parameterize quantification model**.

The **Spectra overlay**, **Data preprocessing**, **Wavelength range** and **Loading plot** areas are available.

2 Defining data preprocessing

- Add data preprocessings in the **Data preprocessing** area by clicking on . By clicking on and , lines can be moved up or down and thus the order of application can be set.
- In the **Data preprocessing** field, select the type of data preprocessing and fill in the associated fields.

Optionally, data preprocessings can be added automatically with the **[Optimize parameterization]** function. Additional information on this in step 4 **Optimize parameterization**.

Additional information on different data preprocessings and their parameters: *(see "Data preprocessing – Area", chapter 5.13.1.17, page 1100)*

The preprocessed spectra are shown immediately in the **Spectra overlay** area.

3 Defining the wavelength range

- Add wavelength ranges in the **Wavelength range** area by clicking on .
- Define the wavelength range manually:
  - Define the start wavelength in the **Start wavelength** column for each wavelength range.
  - Define the end wavelength in the **End wavelength** column for each wavelength range.

  or

- Define the wavelength range using the **Spectra overlay** area:
  - Click on the desired wavelength range in the **Wavelength range** area.
  - Click on **[Activate moving]** in the **Spectra overlay** area.
  - Move the cursor to the left edge of the highlighted area until the cursor is displayed as .
  - Hold down the left mouse button and move the left edge as desired.
  - Proceed in the same way on the right side of the highlighted area.
  - To move a wavelength range, move the cursor over the area until the cursor is displayed as . Hold down the left mouse button and move the area as desired.

- The wavelength ranges may not overlap.
- A minimum difference of 5 nm between start wavelength and end wavelength must be observed.

When defining the wavelength range in the **Spectra overlay** area, the values in the fields of the **Wavelength range** area are automatically adjusted.

Optionally, wavelength ranges can be defined automatically with the **[Optimize parameterization]** function. Additional information on this in step 4 **Optimize parameterization**.

The definition of the start wavelengths and end wavelengths is immediately displayed in the **Spectra overlay** area.

4 Optimize parameterization (optional)

Automatic definition or optimization of data preprocessing and wavelength range

- Automatically define or optimize data preprocessings and wavelength ranges in the **Spectra overlay** and **Loading plot** area by clicking on the **[Optimize parameterization]** button.
  Note: If no data preprocessings or wavelength ranges have previously been defined, then the **[Optimize parameterization]** function will automatically define the best possible data preprocessings and wavelength ranges.
  Note: If data preprocessings or wavelength ranges have already been defined manually, then the **[Optimize parameterization]** function will recalculate and reoptimize the existing values. The existing values are overwritten.

Additional information on different data preprocessings and their parameters: *(see "Data preprocessing – Area", chapter 5.13.1.17, page 1100)*

The preprocessed spectra as well as the start wavelengths and end wavelengths are displayed immediately in the **Spectra overlay** area and not until after calculation of the quantification model in the **Loading plot** area.

5 Calculating the quantification model

- Click on **[Calculate]** to calculate the quantification model.

For large spectra lists, this step may take some time, especially when using the **Leave-One-Out** cross-validation method.

If the **[Calculate]** button is disabled, then the following causes may apply:

- The quantification model has already been calculated and has not been changed since then.
- An incorrect entry was made in one of the process steps. The process step of the affected area is displayed in **red** in the navigator. The field with the incorrect entry is outlined in red.

6 Loading plot

- To check the selected wavelength ranges and the selected number of latent variables, select the **Loading plot** area in the selection list.
- Show or hide the loadings of the latent variables (LV) via the check boxes. High values for the intensity point to important wavelength ranges.

- If the wavelength ranges need to be adjusted, this can be done either in the **Wavelength range** or **Spectra overlay** area or directly in the **Loading plot**. Changes in one of these areas are displayed in the other 2 areas at the same time.

After changing the wavelength range, the data in the displayed **Loading plot** in the **Parameterize quantification model** step is no longer up to date. The quantification model must be calculated once again in order to display up-to-date data in the **Loading plot**.

Additional information on the Loading plot: *(see "Loading plot – Area", chapter 5.13.1.22, page 1113)*

Validating the quantification model

Prerequisite:

- The **Models** ▶ **Quantification models** subsection is opened.
- A quantification model is open and at the front.
- All actions in the **Select samples** process step have been executed.
- The quantification model has been calculated.

1 Change to the "Validate quantification model" process step

- In the navigator, change to the next process step of editing the quantification model by clicking on **Validate quantification model**.

The **Figures of merit**, **Correlation plot**, **Loading plot**, **Influence plot** and **Score plot** areas are available.

2 Rating and editing a quantification model (optional)

Selecting the number of latent variables

- Select the required number of latent variables in **Figures of merit**.
  Make selection based on the chart:
  – In the chart, move the cursor over the green vertical line until the cursor is displayed as ↔.
  – Hold down the left mouse button and move the line horizontally so that the line is above the desired number of variables.

  Make selection based on the table:
  – In the table, double-click on the line with the desired number of variables in the **LV#** column.

    The number of latent variables is indicated by ✓ in the table. If the number of latent variables selected differs from the number suggested by the system, then the suggested number is indicated by →.

The number of latent variables affects the quality of the calculated quantification model.
Additional information on figures of merit: *(see "Figures of merit – Definition", chapter 5.13.1.19, page 1103)*

Correlation plot

- Depending on the number of latent variables, the curve changes as well as the calculated value in **Correlation plot**. This allows the quality of the quantification model to be checked.
- To show or hide outliers, right-click in the chart and select **[Show/hide outliers]** in the context menu.

Additional information on the Correlation plot: *(see "Correlation plot – Area", chapter 5.13.1.20, page 1108)*

Influence plot

- The selected number of latent variables changes the values of the **Hotelling's T²** and **Q residuals** in the **Influence plot**. High values for Hotelling's T² and Q residuals indicate possible outliers.

Additional information on the Influence plot: *(see "Influence plot – Area", chapter 5.13.1.21, page 1112)*

Score plot

- To analyze the relationship between the spectra and detect possible outliers, open the **Score plot** area.
- Select the latent variables for the **x-axis** and **y-axis** in . By default, latent variable 1 is selected for the **x-axis** and latent variable 2 is selected for the **y-axis**.

Additional information on the Score plot: *(see "Score plot – Area", chapter 5.13.1.23, page 1114)*

Loading plot

- To check the selected wavelength ranges and the selected number of latent variables, open the **Loading plot** area.
- Show or hide the loadings of the latent variables (LV) via the check boxes. High values for the intensity point to important wavelength ranges.
- If the wavelength ranges need to be adjusted, this can be done either in the **Wavelength range** or **Spectra overlay** area or directly in the **Loading plot** in the **Parameterize quantification model** step. Additional information on these areas under: *Parameterizing quantification models*

Additional information on the Loading plot: *(see "Loading plot – Area", chapter 5.13.1.22, page 1113)*

Editing the assignment of the spectra to dataset

- To edit the assignment of the spectra to the **Calibration dataset**, **Validation dataset** or **Outlier dataset**, right-click in the chart in the **Influence plot**, **Correlation plot** or **Score plot** area and assign the spectrum to the desired dataset in the context menu.

Any change to the assignment of the spectra (including addition and deletion of spectra) necessitates a recalculation of the quantification model.

The recalculated data is displayed in the **Validate quantification model** process step. The selection of the number of latent variables may have to be performed again (see step 2).

3 Recalculating the quantification model (optional)

- If the changes have been made to the assignment of spectra to the various datasets, or spectra have been added or removed, recalculate the quantification model by clicking on **[Calculate]**.

4 Saving a quantification model

- Save the quantification model by clicking on .

The version and change date of the quantification model are updated automatically in **Properties** ▶ **General**.

5 Publishing a quantification model

- Instructions for publishing quantification models: *(see "Nearest Neighbor Distance – Definition", chapter 5.13.1.10, page 1080), (see "Publishing models", chapter 5.13.1.11, page 1080)*

The quantification model must be published in order to enable its use in determinations and repredictions.

See also

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Creating quantification model (chapter 5.13.1.7, page 1074)

Developing quantification models with OMNIS Model Developer (OMD) (chapter 5.13.1.24, page 1114)

Importing spectra and reference parameters (chapter 5.13.1.14.1, page 1098)

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

Preparing quantification model (chapter 5.13.1.6, page 1069)

Publishing models (chapter 5.13.1.11, page 1080)

Reprocessing a quantification model (chapter 5.13.1.5, page 1068)

Sample list – Tab (chapter 5.2.2, page 159)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.1.13 Pre-calibration – Definition

Pre-calibrations are licensed, ready-to-use quantification models that can be purchased from Metrohm for specific applications (e.g. hydroxyl number in polyols).

Additional information on the licenses can be obtained at the *Metrohm Knowledge Base* or from your regional Metrohm representative.

Pre-calibrations can be imported into the OMNIS Software like quantification models. In addition to the import, a license is required for your use. Instructions for importing a pre-calibration: *(see "Importing models", chapter 5.13.1.8, page 1077)*.

Pre-calibrations are indicated under **Models** ▶ **Quantification models** with the icon.

Pre-calibrations cannot be edited and are used in the OMNIS Software as a **Quantification model type light**. *(see "Models – Definition", chapter 5.13.1.1, page 1056)*

See also

Creating quantification model (chapter 5.13.1.7, page 1074)

Editing quantification model (chapter 5.13.1.12, page 1082)

Importing models (chapter 5.13.1.8, page 1077)

Models – Definition (chapter 5.13.1.1, page 1056)

Quantification models – Subsection (chapter 5.13.1, page 1055)

5.13.1.14 Spectra list – Area

The spectra of the model are displayed in the **Spectra list** area.

- In **Models** ▶ **Quantification models** ▶ **Select samples** ▶ **Spectra list**, the spectra of the quantification model are displayed: *Spectra list in the quantification model*
- In **Models** ▶ **Identification models** ▶ **Select samples** ▶ **Spectra list**, the spectra of the identification model is displayed: *Spectra list in the identification model*

As soon as spectra are selected in the **Spectra list** area, they are highlighted in the **Spectra overlay** area.

Spectra list in the quantification model

The following functions are available:

-

  Use **Edit reference parameter** to edit the reference parameter of the quantification model.

-

  Use **Automatic splitting of dataset** to automatically split the dataset.

-

  Use **Add spectra** to add other spectra to the model.

-

  Use **Delete spectrum** to delete the selected spectra from the model.

The spectra in the spectra list must be split into a calibration dataset and a validation dataset for external validation of the quantification model:

- Spectra assigned to the **calibration dataset** with their reference values serve as the calculation basis of the quantification model.
- Spectra assigned to the **validation dataset** are used with their reference values to validate the quantification model.

- If spectra or reference values are erroneous, they are assigned to the **outlier dataset**. This data is not included in the calculation of the quantification model.

If values of samples included in the quantification model are changed in the sample list, then a message will be displayed in the quantification model. *(see "Reprocessing a quantification model", chapter 5.13.1.5, page 1068), (see "Preparing quantification model", chapter 5.13.1.6, page 1069)*

The following information is displayed in the spectra list:

	The spectrum is assigned to the calibration dataset.
	The spectrum is assigned to the validation dataset.
	The spectrum is assigned to the outlier dataset.
	The subsample from which this spectrum is obtained is available in the OMNIS Software database.
	The subsample from which this spectrum is obtained is not available in the OMNIS Software database. The spectrum and the reference value are only available in the quantification model.
	The spectrum has been imported from an external file.
Sample name	Name of the sample whose spectrum was acquired.
Subsample name	Name of the subsample whose spectrum was acquired.
Source	Name of the command with which the spectrum was acquired or name of the external file from where the spectrum was imported.
Reference parameter/ unit	Value of the reference parameter and its unit, if available.
Determination start	Time point at which the determination was started.

The following information is displayed below the spectra list:

Calibration dataset	The number of spectra that is assigned to the calibration dataset.

Validation dataset	The number of spectra that is assigned to the validation dataset.
Outlier dataset	The number of spectra that is assigned to the outlier dataset.

In the context menu, the following functions are displayed in the spectra list:

	The selected spectra are assigned to the **Calibration dataset**.
	The selected spectra are assigned to the **Validation dataset**.
	The selected spectra are assigned to the **Outlier dataset**.

Spectra list in the identification model

The following functions are available:

-
  Use **Automatic splitting of dataset** to automatically split the dataset.
-
  Use **Add spectra** to add other spectra to the model.
-
  Use **Delete spectrum** to remove the selected spectra from the model.

The spectra in the spectra list must be split into a calibration dataset and a validation dataset for external validation of the identification model:

- Spectra assigned to the **calibration dataset** with their product serve as the calculation basis for the identification model.
- Spectra assigned to the **validation dataset** with their product serve to validate the identification model.
- If spectra or products are erroneous, they are assigned to the **Outlier dataset**. This data is not included in the calculation of the identification model.

If changes are made in the sample list for products contained in the identification model, then no message will be displayed in the identification model.

The following information is displayed in the spectra list:

	The spectrum is assigned to the calibration dataset.

	The spectrum is assigned to the validation dataset.
	The spectrum is assigned to the outlier dataset.
	The subsample from which this spectrum is obtained is available in the OMNIS Software database.
	The subsample from which this spectrum is obtained is not available in the OMNIS Software database. The spectrum and the product are available only in the identification model.
	The spectrum has been imported from an external file.
Sample name	Name of the sample whose spectrum was acquired.
Subsample name	Name of the subsample whose spectrum was acquired.
Source	Name of the command with which the spectrum was acquired or name of the external file from where the spectrum was imported.
Product	Name of the product assigned to the spectrum.
Determination start	Time point at which the determination was started.

In the context menu, the following functions are displayed in the spectra list:

	The selected spectra are assigned to the **Calibration dataset**.
	The selected spectra are assigned to the **Validation dataset**.
	The selected spectra are assigned to the **Outlier dataset**.
Assign product	Opens the **Assign product** dialog where a new product can be assigned to the selected spectra.

Additional information on assigning products in the identification model: *(see "Editing identification model", chapter 5.13.3.5, page 1141)*

See also

Creating quantification model (chapter 5.13.1.7, page 1074)

Editing quantification model (chapter 5.13.1.12, page 1082)

Importing spectra and reference parameters (chapter 5.13.1.14.1, page 1098)

Preparing quantification model (chapter 5.13.1.6, page 1069)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

Reprocessing a quantification model (chapter 5.13.1.5, page 1068)

5.13.1.14.1 Importing spectra and reference parameters

The OMNIS Software enables the import of spectra and their reference parameters from external software systems. Spectra files can be imported from Vision in the NSAS format.

XDS analyzers and DS analyzers with a wavelength range of 400 to 2,500 nm are supported.

Additional information on creating models with NSAS spectra files:

- *(see "Creating quantification model", chapter 5.13.1.7, page 1074)*
- *(see "Creating identification model", chapter 5.13.3.4, page 1139)*

Additional information on adding the NSAS spectra file to an existing model or model hierarchy:

- *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*
- *(see "Editing identification model", chapter 5.13.3.5, page 1141)*
- *(see "Creating and editing a model hierarchy", chapter 5.13.4.3, page 1161)*

See also

Identification model – Tab (chapter 5.13.3.1, page 1129)

Preparing identification model (chapter 5.13.3.3, page 1135)

Preparing quantification model (chapter 5.13.1.6, page 1069)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

Reprocessing a quantification model (chapter 5.13.1.5, page 1068)

5.13.1.15 Histogram – Area

The distribution of the spectra with respect to a certain reference value is shown in **Models** ▶ **Quantification models** ▶ **Select samples** ▶ **Histogram**. 10 equal-sized bins (this value is called **bin number** in Microsoft Excel) are always defined to display the frequency of the reference values in **Histogram**. The bin height corresponds to the number of reference values within the respective interval.

Additional information on editing a quantification model: *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*

As soon as the **Automatic splitting of dataset** function has been executed or datasets have been split manually, the bins of the histogram are displayed in color according to the assignment of the datasets:

Blue	Spectra that are assigned to a **calibration dataset**.
Green	Spectra that are assigned to the **validation dataset**.
Red	Spectra that are assigned to the **outlier dataset**.

See also

Editing quantification model (chapter 5.13.1.12, page 1082)

Models – Definition (chapter 5.13.1.1, page 1056)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

Spectra list – Area (chapter 5.13.1.14, page 1094)

Spectra overlay – Area (chapter 5.13.1.16, page 1099)

5.13.1.16 Spectra overlay – Area

All spectra of the spectra list are shown overlaid in the **Spectra overlay** area. The **Spectra overlay** is used in the following subsections:

- Under **Models** ▶ **Quantification models** in the **Select samples** and **Parameterize quantification model** process steps
- Under **Models** ▶ **Identification models** in the **Select samples** and **Parameterize identification model** process steps

Spectra overlay

The raw spectra are displayed in the **Select samples** process step. Once a spectrum is selected in the spectra list area, the spectrum is highlighted in the **Spectra overlay** area.

In the **Parameterize quantification model** or **Parameterize identification model** process step, defined wavelength ranges are displayed in the **Spectra overlay** area. The start wavelength and end wavelength of the wavelength ranges are adjusted in the **Spectra overlay** area. The spectra are displayed with data preprocessing applied.

For quantification models, data preprocessings and wavelength ranges can be automatically calculated or optimized using the **[Optimize parameterization]** function.

Additional information on defining wavelength ranges:

- For quantification models: *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*
- For identification models: *(see "Editing identification model", chapter 5.13.3.5, page 1141)*

Spectra in the **Identification model** are marked with different color codings. A distinction is made between 2 types:

- **Colors of the datasets**
  In the **Spectra overlay** area, spectra in the calibration dataset are marked **blue**, spectra in the validation dataset are marked **green** and spectra in the outlier dataset are marked **red**.
- **Product colors**
  The product colors defined in the **Product list** area are used to display spectra in the **Spectra overlay** area.

The **Spectra overlay** areas in the **Select samples** and **Parameterize identification model** process steps are not synchronized and can exhibit different types of color coding.

Product colors are disabled by default and the colors of the datasets are used.
Additional information on product colors: *(see "Product list – Area", chapter 5.13.3.6, page 1150)*
Additional information on the activation of product colors: *(see "Identification model – Tab", chapter 5.13.3.1, page 1129)*

See also

Data preprocessing – Area (chapter 5.13.1.17, page 1100)

Editing identification model (chapter 5.13.3.5, page 1141)

Editing quantification model (chapter 5.13.1.12, page 1082)

Wavelength range – Area (chapter 5.13.1.18, page 1102)

5.13.1.17 Data preprocessing – Area

Data preprocessings are defined in the **Data preprocessing** area.

- Data preprocessings for an open quantification model can be defined manually or automatically under **Models** ▶ **Quantification models** ▶ **Parameterize quantification model** ▶ **Data preprocessing**. The data preprocessings are used for the calculation of the quantification model as well as for the **PREDICT** command that refers to the quantification model. *(see "PREDICT – Parameters", chapter 5.11.8.16, page 610)*

- Data preprocessings for an open identification model are defined in **Models** ▶ **Identification models** ▶ **Parameterize identification model** ▶ **Data preprocessing**. The data preprocessings are used for the calculation of the identification model as well as for the **PREDICT** command that refers to the identification model. *(see "PREDICT – Parameters", chapter 5.11.8.16, page 610)*
- In **Processes** ▶ **Methods** ▶ **EVAL BASE STATISTICS** ▶ **Properties** ▶ **Parameters**, data preprocessings for a **EVAL BASE STATISTICS** command are defined. *(see "EVAL BASE STATISTICS – Parameters", chapter 5.11.8.67, page 773)*

Defining data preprocessings

Clicking on adds data preprocessings individually and clicking on removes them again. By clicking on or , data preprocessings can be moved up or down. This changes the sequence in which the data preprocessings are applied. A maximum of 10 data preprocessing steps can be added.

Alternatively, data preprocessings can be added with **[Add data preprocessing]** and deleted with **[Remove data preprocessing]** in the context menu.

Data preprocessings for quantification models can be automatically defined using the **[Optimize parameterization]** function. If no data preprocessings were previously defined, then select the **[Optimize parameterization]** function to automatically define the best possible data preprocessings. If data preprocessings have been defined, then the **[Optimize parameterization]** function recalculates and reoptimizes the existing values.

Additional information on optimization of data preprocessings: *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*

Parameters of the data preprocessings

4 data preprocessings are available in the OMNIS Software: **Detrend**, **Gap-Segment**, **Savitzky-Golay** and **SNV**.

Detrend	
Correction of the baseline drift. If **Detrend** is selected, then the following specific parameters appear:	
Start wavelength	Define the lower limit of the wavelength range. **Note**: A minimum of 5 nm distance must be observed between the start wavelength and the end wavelength.
End wavelength	Define the upper limit of the wavelength range.

Gap-Segment	

Derivative of the spectrum. The measuring points of 2 segments, which are separated by a gap, are incorporated in the derivative.

If **Gap-Segment** is selected, then the following specific parameters appear:

Derivative order	Specification as to how often the spectrum is to be derived.
Segment size	Define the segment size.
Gap size	Define the gap between the 2 segments.

Savitzky-Golay	
Smoothing and derivative of the spectrum with a Savitzky-Golay filter.	
If **Savitzky-Golay** is selected, then the following specific parameters appear:	
Derivative order	Specification as to how often the spectrum is to be derived.
Filter width	Define the filter width of the Savitzky-Golay filter.
Polynomial degree	Define the polynomial degree of the Savitzky-Golay filter.

SNV (standard normal variate)	
Standardizing the spectrum with the variance.	
If **SNV** is selected, then the following specific parameters appear:	
Start wavelength	Define the lower limit of the wavelength range. **Note**: A minimum of 5 nm distance must be observed between the start wavelength and the end wavelength.
End wavelength	Define the upper limit of the wavelength range.

See also

EVAL BASE STATISTICS – Parameters (chapter 5.11.8.67, page 773)

Editing quantification model (chapter 5.13.1.12, page 1082)

Models – Definition (chapter 5.13.1.1, page 1056)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

Quantification models – Subsection (chapter 5.13.1, page 1055)

Spectra overlay – Area (chapter 5.13.1.16, page 1099)

Wavelength range – Area (chapter 5.13.1.18, page 1102)

5.13.1.18 Wavelength range – Area

Wavelength ranges are defined in the **Wavelength range** area.

- Wavelength ranges for an open quantification model are defined manually or automatically under **Models** ▶ **Quantification models** ▶ **Parameterize quantification model** ▶ **Wavelength range**.

- Wavelength ranges for an open identification model are defined under **Models** ▶ **Identification models** ▶ **Parameterize identification model** ▶ **Wavelength range**.
- In **Processes** ▶ **Methods** ▶ **EVAL BASE STATISTICS** ▶ **Properties** ▶ **Parameters**, wavelength ranges for a **EVAL BASE STATISTICS** command are defined. *(see "EVAL BASE STATISTICS – Parameters", chapter 5.11.8.67, page 773)*

Determining wavelength ranges

Clicking on adds wavelength ranges individually and clicking on deletes them again. Up to 10 wavelength ranges can be defined.

Wavelength ranges can be automatically optimized for quantification models using the **[Optimize parameterization]** function in the **Spectra overlay** or **Loading plot** area.

- Additional information on editing the quantification model: *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*
- Additional information on editing the identification model: *(see "Editing identification model", chapter 5.13.3.5, page 1141)*

Parameters of the wavelength ranges

Start wavelength	Enter the lower limit of the wavelength range. **Note**: A minimum of 5 nm distance must be observed between the start wavelength and the end wavelength. **Note**: The wavelength ranges may not overlap.
End wavelength	Enter the upper limit of the wavelength range.

See also

Data preprocessing – Area (chapter 5.13.1.17, page 1100)

EVAL BASE STATISTICS – Parameters (chapter 5.11.8.67, page 773)

Models – Definition (chapter 5.13.1.1, page 1056)

Spectra overlay – Area (chapter 5.13.1.16, page 1099)

5.13.1.19 Figures of merit – Definition

The figures of merit of the quantification model are displayed in the **Figures of merit** area. Based on the figures of merit, it is possible to select the optimal number of latent variables. The figures of merit determine the error that can be expected for the prediction of unknown samples.

The following values are displayed in the **Figures of merit** area:

Number of latent variables

A quantification model maps the measuring points of the spectra or associated reference values with a specific number. The selection of the number of latent variables is crucial for good predictive ability. Too few or too many latent variables lead to inaccurate predictions: If too few latent variables are considered, then the variance of the samples will be described incompletely. If too many latent variables are selected, then the quantification model will describe sample-unspecific variance, which is caused, for example, by instrument noise.

Standard error of calibration

The standard error of calibration **SEC** shows the standard deviation between the reference value and the calculated value based on the calibration data set. A low standard error of calibration indicates that the calibration describes the calibration dataset well, but says nothing about the prediction quality for unknown samples.

$$\mathrm{SEC} = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n-k-1}}$$

Here *i* corresponds to the sample from the calibration data set, $\hat{y}_i$ corresponds to the estimated value of *i*, y_i corresponds to the reference value of *i*, n corresponds to the number of samples from the calibration dataset and k corresponds to the number of latent variables.

Standard error of cross-validation

The standard error of cross-validation calibration **SECV** shows the standard deviation between the reference value and the calculated value based on the calibration data set. The standard error is determined by cross-validation:

$$\mathrm{SECV} = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n}}$$

Here *i* corresponds to the sample, $\hat{y}_i$ corresponds to the estimated cross-validation of *i*, y_i corresponds to the reference value of *i*, and n corresponds to the number of all samples used to develop the quantification model.

Coefficient of determination of cross-validation

The coefficient of determination of the cross-validation **R^2CV** shows the correlation of the reference value and the calculated value. The coefficient of determination is determined by cross-validating all samples used to develop the quantification model:

$$r^2_{y,\hat{y}} = \frac{(\sum_{i=1}^{n}(y_i - \bar{y}_i) \cdot (\hat{y}_i - \bar{\hat{y}}_i))^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2 \cdot \sum_{i=1}^{n}(\hat{y}_i - \bar{\hat{y}}_i)^2}$$

Here *i* corresponds to the sample, y_i corresponds to the reference value of *i*, $\bar{y}$ corresponds to the mean value of the reference values, $\hat{y}_i$ corresponds to the estimated cross-validation of *i*, $\bar{\hat{y}}$ corresponds to the mean value of the calculated values, and n corresponds to the number of all samples used to develop the quantification model.

The higher the number of latent variables, the more variance can be explained by the model. If possible, the number of latent variables should be chosen so that the ratio is SECV : SEC = 1.2 : 1. Another indication of the optimal selection of latent variables is the first minimum of the SECV value. A correlation greater than 0.95 should be aimed for.

Standard error of prediction

The standard error of prediction **SEP** shows the standard deviation between the reference value and the calculated value based on the validation dataset:

$$\mathrm{SEP} = \sqrt{\frac{\sum_{i=1}^{v}(\hat{\mathrm{v}}_i - \mathrm{v}_i)^2}{v}}$$

Here *i* corresponds to the sample from the validation dataset, $\hat{\mathrm{v}}_i$ corresponds to the calculated value of *i*, v_i corresponds to the reference value of *i*, and v corresponds to the number of samples from the validation dataset.

Coefficient of determination of prediction

The coefficient of determination of the prediction **R²P** shows the correlation of the reference value and the calculated value, based on the validation dataset:

$$r^2_{y,\hat{y}} = \frac{(\sum_{i=1}^{v}(y_i - \bar{y}_i) \cdot (\hat{y}_i - \bar{\hat{y}}_i))^2}{\sum_{i=1}^{v}(y_i - \bar{y}_i)^2 \cdot \sum_{i=1}^{v}(\hat{y}_i - \bar{\hat{y}}_i)^2}$$

Here *i* corresponds to the sample, y_i corresponds to the reference value of *i*, $\bar{y}$ corresponds to the mean value of the reference values, $\hat{y}_i$ corresponds to the estimated cross-validation of *i*, $\bar{\hat{y}}$ corresponds to the mean value of the calculated values, and v corresponds to the number of samples from the validation dataset.

The higher the number of latent variables, the more variance can be explained by the model. If possible, the number of latent variables should be chosen so that the ratio is SECV : SEC = 1.2 : 1. Another indication of

the optimal selection of latent variables is the first minimum of the SECV value. A correlation greater than 0.95 should be aimed for.

See also

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Editing quantification model (chapter 5.13.1.12, page 1082)

Influence plot – Area (chapter 5.13.1.21, page 1112)

Models – Definition (chapter 5.13.1.1, page 1056)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

5.13.1.19.1 Figures of merit – Area

The figures of merit are displayed as a chart and as a table in **Models ▶ Quantification models ▶ Validate quantification model ▶ Figures of merit**. Depending on whether the quantification model was calculated with a validation dataset, the **SEC. SECV** or **SEC. SECV. SEP** measured quantities are displayed on the y-axis of the chart.

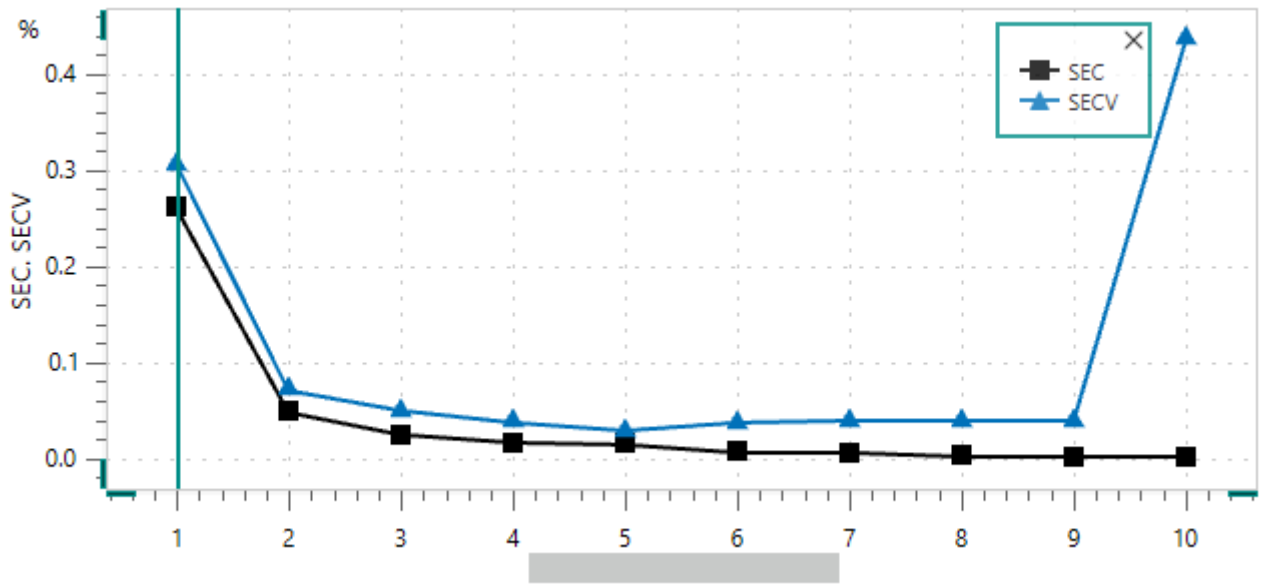
Display of the figures of merit

The green vertical line indicates the currently selected number of latent variables. By clicking and moving this line in the chart, the number of latent variables can be edited. The selection is displayed in the table. The selection of a number of latent variables can also be made by double-clicking on a line in the table.

If a number of latent variables other than the suggested number is selected, this is indicated in the first column of the table:

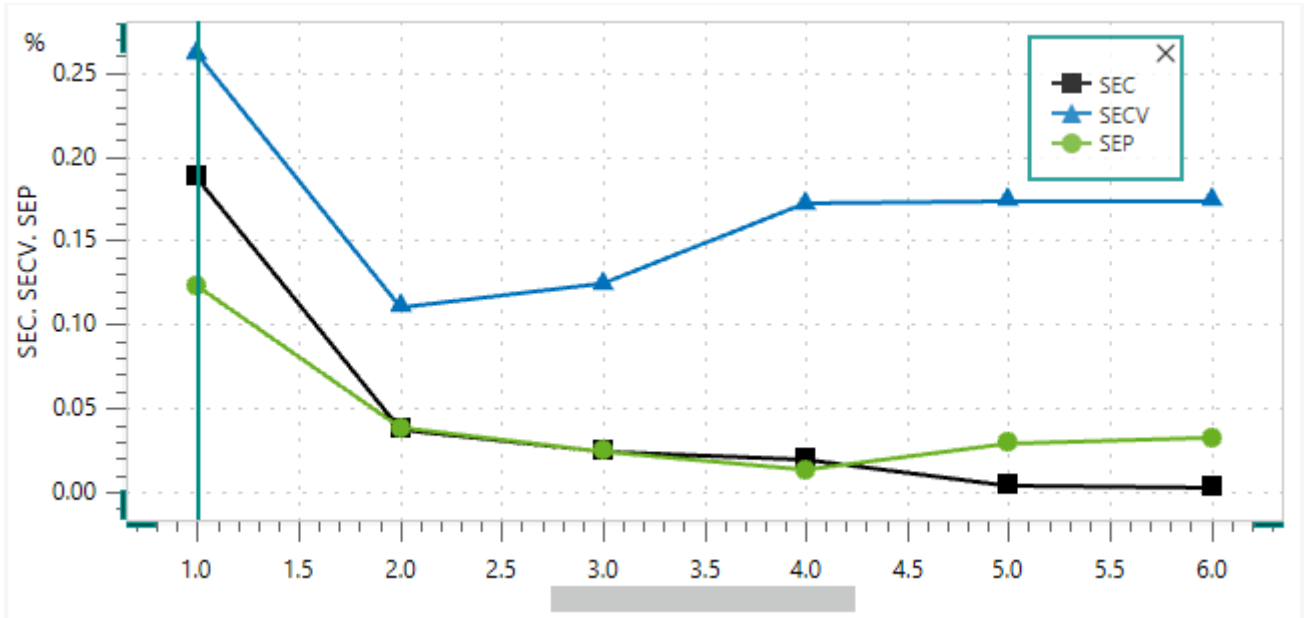
✓	Selected number of latent variables.
→	Suggested number of latent variables.

If no validation dataset has been defined, the following coefficients are displayed in the chart and the table:



Without validation dataset	
LV#	Number of latent variables.
SEC	Standard error of calibration.
SECV	Standard error of cross-validation.
R²CV	Coefficient of determination of cross-validation.

If a validation dataset has been defined, then the following coefficients are displayed in the chart and the table:



With validation dataset	
LV#	Number of latent variables.
SEC	Standard error of calibration.
SECV	Standard error of cross-validation.
SEP	Standard error of prediction.
R²P	Coefficient of determination of prediction.

Additional information on the terms **LV#**, **SEC**, **SECV**, **SEP**, **R²P**:
(see "Figures of merit – Definition", chapter 5.13.1.19, page 1103)

See also

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Editing quantification model (chapter 5.13.1.12, page 1082)

Influence plot – Area (chapter 5.13.1.21, page 1112)

Models – Definition (chapter 5.13.1.1, page 1056)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

5.13.1.20 Correlation plot – Area

The **Correlation plot** graphically displays the correlation between **Reference value** and **Calculated value**. The **Correlation plot** is used in 2 subsections:

- Under **Models** in an open quantification model, the slope and the y-axis intercept value of the regression lines are displayed under **Validate quantification model** ▶ **Correlation plot**: *Correlation plot in the quantification model*
- Under **Slope/y-intercept corrections** for the creation of a slope/y-intercept correction, the correlation between the reference value from the primary method and the calculated or corrected value is displayed in **Correlation plot**: *Correlation plot in slope/y-intercept correction*

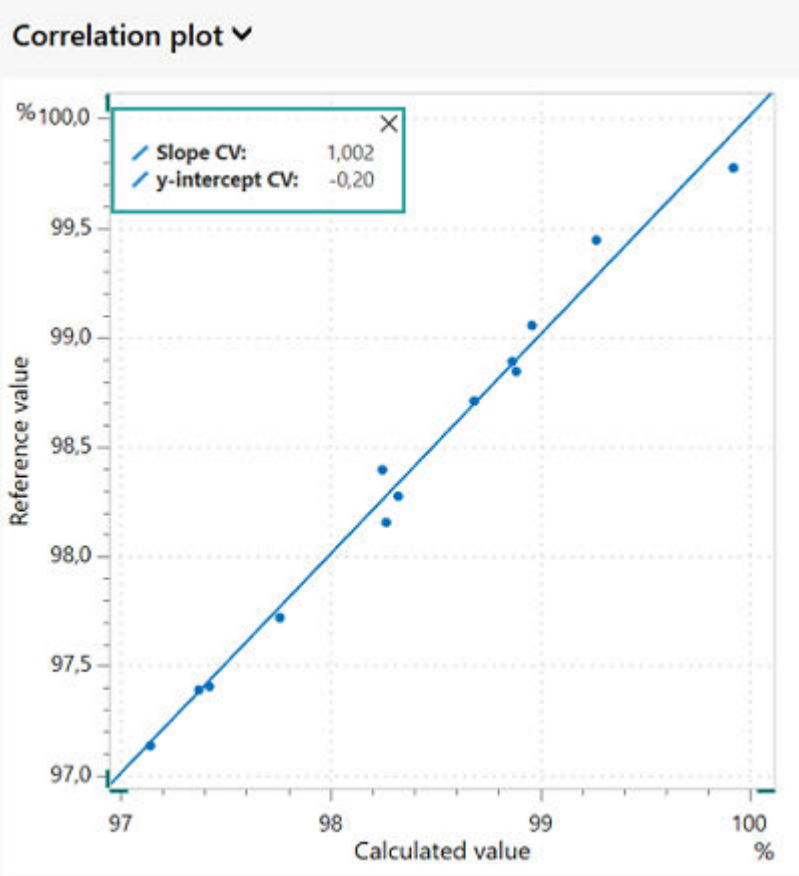
Correlation plot in the quantification model

Under **Validate quantification model**, the values are displayed as a chart and as a table in the **Correlation plot** area. The spectra of the calibration data set are displayed in **blue**, the spectra of the validation data set in **green** and the spectra of the outlier data set in **red**. Outliers have no influence on the calculation of the regression lines.

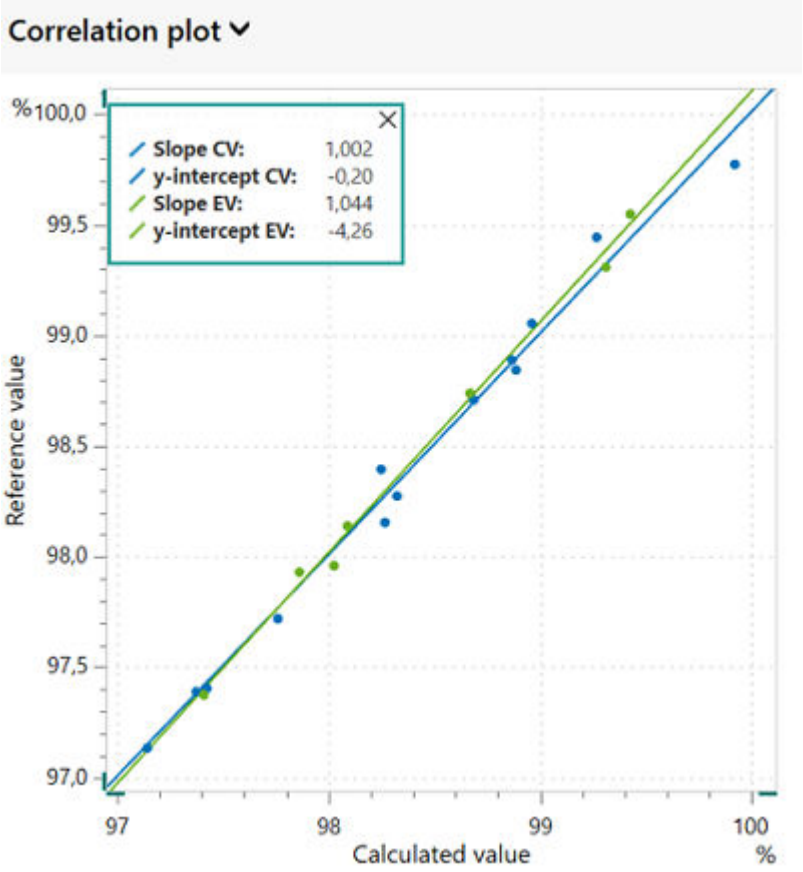
If a validation dataset is used in the creation of the quantification model, then the values of the regression line are also specified separately for this dataset. All calculated values in the correlation plot are determined by the model.

The following values are displayed in the chart:

Quantification model with calibration dataset (without validation dataset)	
Slope CV	Slope of the regression line.
y-intercept CV	y-intercept of the regression line.



Quantification model with calibration dataset and validation dataset	
Slope CV	Slope of the regression line based on the calibration dataset.
y-intercept CV	y-intercept of the regression line based on the calibration data set.
Slope EV	Slope of the regression line based on the validation data set.
y-intercept EV	y-intercept of the regression line based on the validation data set.



To exclude outliers from the calculation, right-click on a point in the chart to open the context menu and then select **[Outlier dataset]**. The quantification model must be calculated again afterwards.

The following values are displayed in the table:

Sample name	Name of the sample to which the spectrum belongs.
Subsample name	Name of the subsample to which the spectrum belongs.
Reference value	Value of the reference parameter applied from the primary method.
Calculated value	▪ Calculated value determined for the calibration dataset. ▪ Calculated value determined for the validation dataset.
Residual	Difference between calculated value and reference value.

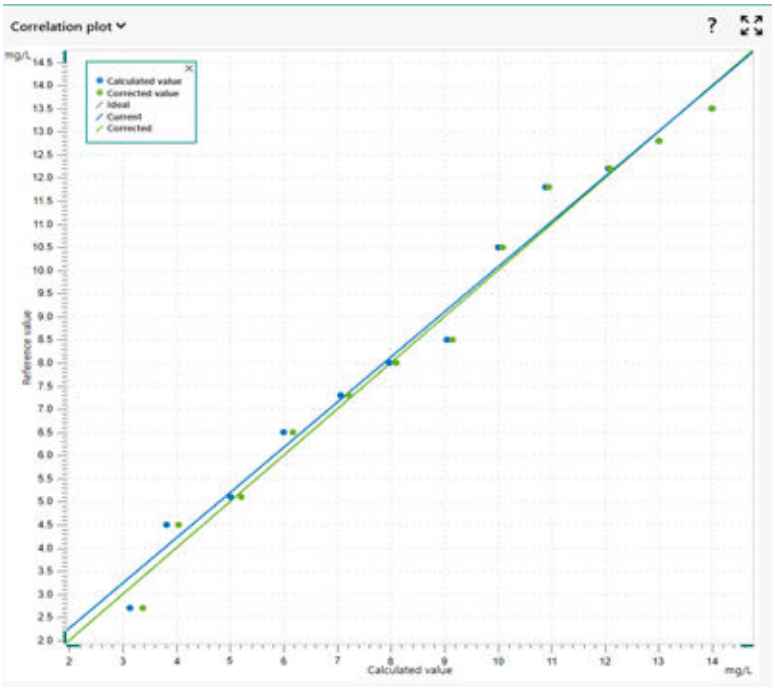
These values are additionally displayed as a details window as soon as the cursor is positioned over a point in the chart.

Correlation plot in the slope/y-intercept correction

The values are displayed as a table and chart in the **Correlation plot** area when the slope/y-intercept correction is created. These values change, depending on whether **Bias** or **Slope/y-intercept** was selected.

The following values are displayed in the chart, depending on the selection of the correction:

Calculated value	Value that was calculated by applying the quantification model to the spectrum.
Corrected value	Calculated value that was corrected with the bias correction or slope/y-intercept correction.
Ideal	Ideal line of the regression line with slope = 1 and y-intercept = 0.
Current	Regression line of the values that was calculated by applying the quantification model to the spectrum.
Corrected	Regression line after applying the slope/y-intercept correction or the bias correction.



The following values are displayed in the Details window of the chart:

Reference value	Value of the reference parameter taken from the primary method.

Calculated value	Value that was calculated by using the quantification model on the spectrum.
Corrected value	Value that was corrected to the calculated value by using the bias correction or slope/y-intercept correction.
Residual	▪ For the blue points: Difference between calculated value and reference value. ▪ For the green points: Difference between corrected value and reference value.

To exclude outliers from the calculation, right-click on an entry in the **Samples** area to open the context menu and then select **[Mark sample as outlier]**.

Additional information on creating a slope/y-intercept correction: *(see "Creating a slope/y-intercept correction", chapter 5.13.2.3, page 1120)*

See also

Editing quantification model (chapter 5.13.1.12, page 1082)

Figures of merit – Area (chapter 5.13.1.19.1, page 1106)

Histogram – Area (chapter 5.13.1.15, page 1098)

Influence plot – Area (chapter 5.13.1.21, page 1112)

5.13.1.21 Influence plot – Area

Possible outliers of the dataset after the application of the selected data preprocessing and the chosen wavelength selection are displayed under **Models** ▶ **Quantification models** ▶ **Validate quantification model** ▶ **Influence plot**. **PLS** and **PCA** are available as calculation methods.

The distribution of the data sets as a value pair of **Hotelling's T²** and **Q residuals** is displayed in the chart. High values for **Hotelling's T²** and **Q residuals** indicate possible outliers. The significance level is displayed with 2 dashed lines so that spectra can be recognized as outliers more easily.

The significance level is defined under **Select samples** ▶ **Properties** ▶ **Outlier limits** ▶ **Significance level**.

Additional information on the significance level: *(see "Significance level – Definition", chapter 5.13.1.25, page 1117)*

Outliers are highlighted in red. Outliers can be added or changed manually. Spectra or reference values can be assigned manually to the outlier dataset, if necessary. To do so, right-click a point in the chart to open the context menu and select **[Outlier dataset]**. Multiple points can be

assigned to the dataset at the same time by pressing **[CTRL]** and clicking on additional points.

See also

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Editing quantification model (chapter 5.13.1.12, page 1082)

Figures of merit – Area (chapter 5.13.1.19.1, page 1106)

Quantification model – Properties (chapter 5.13.1.4, page 1065)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

Quantification models – Subsection (chapter 5.13.1, page 1055)

Significance level – Definition (chapter 5.13.1.25, page 1117)

5.13.1.22 Loading plot – Area

The **Loading plot** area can be displayed in an open quantification model in the **Validate quantification model** and **Parameterize quantification model** process steps.

Information for selecting the appropriate wavelength ranges for a quantification model is displayed in **Loading plot**. In addition, the **Loading plot** can be used to verify the selected number of latent variables.

The chart shows the loadings of the latent variables (**LV**) calculated in the quantification model. The latent variables correspond to the various principal components of the quantification model. The display of the loadings can be adjusted by using the check boxes to show or hide loadings. A change in the loadings in one of the loading plots is simultaneously displayed in the other **Loading plot**.

The wavelength ranges that have a correlation with the reference parameters can be identified on the basis of the intensity of the loadings. High values for the intensity point to important wavelength ranges. Wavelength ranges can be defined directly in the **Loading plot** area as well as in other **Wavelength range** and **Spectra overlay** areas in the **Parameterize quantification model** process step.

The **Optimize parameterization** function is used to optimize data preprocessings and wavelength ranges for the creation of the quantification model. The preprocessed spectra and defined wavelengths are not displayed in the **Loading plot** area until after the quantification model has been calculated.

Information on defining wavelength ranges in the **Parameterize quantification model** step: *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*

See also

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Editing quantification model (chapter 5.13.1.12, page 1082)

Figures of merit – Area (chapter 5.13.1.19.1, page 1106)

Quantification model – Tab (chapter 5.13.1.2, page 1059)

Spectra overlay – Area (chapter 5.13.1.16, page 1099)

Wavelength range – Area (chapter 5.13.1.18, page 1102)

5.13.1.23 Score plot – Area

The **Score plot** area is displayed in a quantification model in **Validate quantification model**.

A score plot represents the distribution of the spectra in a chart. Using the groupings of the spectra in the chart, the relationship between the spectra can be analyzed and possible outliers can be recognized. The scores are determined using the PLS calculation method.

The latent variables for the **x-axis** and **y-axis** are selected in . Depending on this selection, the scores of the spectra for the latent variables are displayed.

By default, latent variable 1 is selected for the **x-axis** and latent variable 2 is selected for the **y-axis**.

Outliers are highlighted in red in the score plot. To add outliers manually or to select a different type of dataset for a spectrum, right-click on a point in the chart to open the context menu. Then select the desired dataset. Multiple points can be assigned to the dataset at the same time by pressing **[CTRL]** and clicking on additional points.

See also

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Editing quantification model (chapter 5.13.1.12, page 1082)

Figures of merit – Area (chapter 5.13.1.19.1, page 1106)

Influence plot – Area (chapter 5.13.1.21, page 1112)

Loading plot – Area (chapter 5.13.1.22, page 1113)

Spectra list – Area (chapter 5.13.1.14, page 1094)

5.13.1.24 Developing quantification models with OMNIS Model Developer (OMD)

The OMNIS Model Developer (OMD) enables the automatic development of quantification models.

The OMD creates 5 quantification models from the selected samples, each of which has a different predictive ability. Each of these 5 calculated mod-

els can be used for evaluation of the samples. If needed, these quantification models can be edited further prior to publishing.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Executing OMNIS Model Developer

The OMD can be started in the following ways:

- In the last step of the creation of the quantification model: *(see "Creating quantification model", chapter 5.13.1.7, page 1074)*
  or
- After the creation in the opened quantification model:
  – Open the required quantification model in **Models ▶ Quantification models**.
  – Click on **[Start OMD]**.

The duration of the OMD execution depends on the number of spectra.

If tags are assigned to a quantification model that has already been created, and if it is calculated with the OMD, then the tags for the newly calculated quantification models will be retained.

2 Checking and selecting calculated quantification models

- Enter the desired name of the quantification model in the **Name of the quantification model** field.
- Enter the desired number of **Decimal places** that will be displayed in the results of the quantification model.
- Observe the following information:
  The display shows 5 quantification models that were calculated with the OMD. Clicking on the individual models causes the associated Correlation plot to be displayed.
  The quantification models are sorted according to their predictive ability.

If a quantification model can be improved even further, then suggestions for its improvement will be displayed in the tooltip for the model.

The following colors are used to distinguish between the models:

The predictive ability of the models marked in **green** have a good predictive ability and can be used for the prediction.

The predictive ability of the models marked in **yellow** are not optimal.

The predictive ability of the models marked in **red** do not have sufficient predictive ability and should not be used for the prediction.

3 Editing or publishing quantification models

Later steps depend on whether the OMD was started during the last step at the time of creation or in the opened quantification model. The option of saving and publishing the model directly after the OMD execution occurs only at the time the model is created.

- Click on **[Edit]** if one or more quantification models are still to be edited or if the OMD was started in an opened model.
  - The selected quantification models are opened in separate tabs and can be edited as needed. Additional information on editing quantification models: *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*
  - Save the selected quantification model by clicking on . The version and change date of the quantification model are updated automatically in **Properties** ► **General**.
  - Publish the quantification model. Additional information on publishing quantification models: *(see "Nearest Neighbor Distance – Definition", chapter 5.13.1.10, page 1080), (see "Publishing models", chapter 5.13.1.11, page 1080)*

  or
- If the OMD was started at the time of the creation of the quantification model, then only one quantification model can be selected, and only one can be saved and published. When this is the case, select a model and click on **[Save and publish]**. The other 4 models are discarded.

The quantification model must be published in order to enable its use in determinations and repredictions.

See also

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Creating quantification model (chapter 5.13.1.7, page 1074)

Editing quantification model (chapter 5.13.1.12, page 1082)

Importing spectra and reference parameters (chapter 5.13.1.14.1, page 1098)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

Pre-calibration – Definition (chapter 5.13.1.13, page 1093)

Preparing quantification model (chapter 5.13.1.6, page 1069)

Publishing models (chapter 5.13.1.11, page 1080)

Reprocessing a quantification model (chapter 5.13.1.5, page 1068)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.1.25 Significance level – Definition

The significance level defines the confidence interval for the evaluation of **Q residuals** vs. **Hotelling's T²**. The confidence intervals are displayed in the **Influence plot** area. Spectra which lie outside the confidence interval are possible outliers. The greater the significance level, the more possible outliers are recognized.

The significance level is used in the following areas in the OMNIS Software:

- Quantification models
- Automatic dataset splitting for identification models

Additional information on the significance level for quantification methods: *(see "Editing quantification model", chapter 5.13.1.12, page 1082)*

Additional information on the significance level for identification methods: *(see "Editing identification model", chapter 5.13.3.5, page 1141)*

See also

Models – Definition (chapter 5.13.1.1, page 1056)

5.13.2 Slope/y-intercept corrections – Subsection

The following functions are available in **Models** ▶ **Slope/y-intercept corrections**:

- Use **Create slope/y-intercept correction** to create a new slope/y-intercept correction. A slope/y-intercept correction can be used to correct quantification models or the results of a **PREDICT** command.
- Use **Import slope/y-intercept correction** to import an OSIC file (**O**MNIS **S**lope/y-**I**ntercept **C**orrection) as a slope/y-intercept correction.
- Use **Export slope/y-intercept corrections** to export the selected slope/y-intercept corrections as OSIC files (**O**MNIS **S**lope/y-**I**ntercept **C**orrection).

-
  Reports for the selected slope/y-intercept corrections are generated with **Generate report**. The reports can be saved as a PDF file or also printed out.
-
  The properties of the selected slope/y-intercept correction are displayed in the **Properties** window.
-
  The selected slope/y-intercept corrections are deleted with **Delete slope/y-intercept corrections**.

Overview list

The following information is displayed in the overview list:

Name	Name of the slope/y-intercept correction. The name can be adapted only when creating the slope/y-intercept correction.
Quantification model used	The quantification model for which the slope/y-intercept correction was calculated.
Reference parameter / unit	Reference parameter and unit of the quantification model.
Slope	Calculated slope coefficient of the slope/y-intercept correction.
y-intercept	Calculated y-intercept coefficient of the slope/y-intercept correction.
Saved	Time at which the slope/y-intercept correction was saved.

As soon as the slope/y-intercept correction has been published, it can neither be opened nor edited.

See also

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Exporting slope/y-intercept corrections (chapter 5.13.2.2, page 1119)

Importing a Slope/y-intercept correction (chapter 5.13.2.1, page 1119)

Models – Definition (chapter 5.13.1.1, page 1056)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Reprocessing predictions (chapter 5.10.13.5.1, page 363)

Slope/y-intercept correction – Definition (chapter 5.13.2.6, page 1124)

5.13.2.1 Importing a Slope/y-intercept correction

Prerequisite:

- At least one OMNIS slope/y-intercept correction file (***.osic**) is available.
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting the slope/y-intercept correction

- Click on to open the **Import slope/y-intercept correction** window in **Models** ► **Slope/y-intercept corrections**.

2 Browsing for folder

- Select the folder in which the desired slope/y-intercept correction is saved.

3 Selecting the file

- Select the OMNIS slope/y-intercept correction file or enter the name of the slope/y-intercept correction file in the **File name** field.

4 Confirming and importing the selection

- Click **[Open]** to confirm the selection.

The slope/y-intercept correction is imported into the OMNIS Software.

See also

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Exporting slope/y-intercept corrections (chapter 5.13.2.2, page 1119)

Slope/y-intercept corrections – Subsection (chapter 5.13.2, page 1117)

5.13.2.2 Exporting slope/y-intercept corrections

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- At least one slope/y-intercept correction is available in the overview list.

1 Selecting slope/y-intercept corrections

- Select the desired slope/y-intercept corrections under **Models** ► **Slope/y-intercept corrections**.

- Click on to open the **Export slope/y-intercept corrections** window.

2 Selecting or entering a target folder

- Select the target folder by clicking on or enter the absolute path in the address bar.

3 Creating OMNIS slope/y-intercept correction files

- Export the OMNIS slope/y-intercept correction files (OSIC files) into the target folder by clicking on **[Export]**. One or more OSIC files are exported under the respective name of the slope/y-intercept corrections.
- Click on **[Open target folder]** to open the target folder.

All time indications are converted into Coordinated Universal Time (UTC±00:00) when exporting. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.
The local time on the computer is used for the date and time displayed in the file name.

See also

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Importing a Slope/y-intercept correction (chapter 5.13.2.1, page 1119)

Slope/y-intercept correction – Definition (chapter 5.13.2.6, page 1124)

5.13.2.3 Creating a slope/y-intercept correction

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- At least 10 samples with already predicted reference values and the corresponding reference parameters must be available.

1 Creating a new slope/y-intercept correction

- In **Models** ▶ **Slope/y-intercept corrections**, click on .

2 Entering a name

- Enter the desired name of the slope/y-intercept correction.

The name can be changed in **Slope/y-intercept correction** ▶ **Properties** ▶ **General**. After publishing, the name cannot be changed anymore.

3 Selecting the samples and a quantification model

- Display all the sample lists saved in the database by clicking on **Sample lists**.
  or
- Display all the search queries saved in the database by clicking on **Search queries**.
- Select the sample lists or search queries from which samples are to be used for the creation of the slope/y-intercept correction.
- The **Quantification model, version** list displays all available quantification models of the selected samples.
  Select the quantification model that is to be corrected in this list.
- Click on **[Continue]**.

4 Selecting reference parameters

- If required, change the name of the slope/y-intercept correction.
- The current reference parameter of the quantification model is displayed in the **Reference parameter/unit of the quantification model** field.
- The table displays all available reference parameters of the selected samples.
  In this table, select the same reference parameter as in the quantification model.

If the required reference parameter has several designations in the sample lists or search queries, then all of these designations can be selected.

5 Confirming entries

- Create the new slope/y-intercept correction by clicking on **[Create]**.

Samples with the reference values and the calculated values of the quantification model are applied for the calculation of the slope/y-intercept correction.

6 Selecting the type of correction

- Select the **Bias** option, to calculate the bias.
  or

- Select the **Slope/y-intercept** option, to calculate the slope and the y-intercept.

7 Marking outliers

- To mark the sample as an outlier, right-click on the sample in the **Samples** subsection and select **Mark sample as outlier**.

To not mark the sample as outlier anymore, right-click on the sample again and click on **Remove marking of sample as outlier**.

8 Publishing the slope/y-intercept correction

- Click on .
- Publish the slope/y-intercept correction by clicking on **[Publish and close]**.

A published slope/y-intercept correction can not be opened or edited retrospectively.

The slope/y-intercept correction is published and saved at the same time.

Additional information on the use of slope/y-intercept corrections in determinations and repredictions: *(see "PREDICT – Parameters", chapter 5.11.8.16, page 610)(see "Reprocessing predictions", chapter 5.10.13.5.1, page 363)*

See also

Audit Trail – Directory (chapter 5.14.5, page 1177)

Copying table (chapter 5.2.8, page 172)

Creating quantification model (chapter 5.13.1.7, page 1074)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

Reprocessing predictions (chapter 5.10.13.5.1, page 363)

Slope/y-intercept correction – Definition (chapter 5.13.2.6, page 1124)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.2.4 Slope/y-intercept correction – Properties

Clicking on under **Models** ▶ **Slope/y-intercept corrections** opens the **Properties** window. The following information on the selected slope/y-intercept correction is available in the **General** subsection:

General

Name	Name of the slope/y-intercept correction.
Object ID	Identification number of the slope/y-intercept correction.
Saved	Time at which the slope/y-intercept correction was published.
Saved by	User ID of the user who published the slope/y-intercept correction.

Clicking on under **Models** ▶ **Slope/y-intercept corrections** within an opened slope/y-intercept correction opens the **Properties** window. The following functions and information are available in the **General** subsection:

General

Name	Name of the slope/y-intercept correction (can be edited, max. 255 characters).
Quantification model	Name of the quantification model that is to be corrected.
Reference parameter / unit	Reference parameter and unit of the quantification model that is to be corrected.

See also

Audit Trail – Directory (chapter 5.14.5, page 1177)

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Slope/y-intercept correction – Definition (chapter 5.13.2.6, page 1124)

Slope/y-intercept corrections – Subsection (chapter 5.13.2, page 1117)

5.13.2.5 Correction values – Area

In **Models** ▶ **Slope/y-intercept corrections** ▶ **Slope/y-intercept correction** ▶ **Correction values**, the values **SEP**, **Slope** and **y-intercept** are respectively displayed in a table without correction, with bias correction and with slope/y-intercept correction:

SEP	Standard error of prediction.
Slope	Slope coefficient of the slope/y-intercept correction.
y-intercept	y-intercept coefficient of the slope/y-intercept correction.
Uncorrected	Values without applying a correction.
Bias correction	Values after applying the bias correction.

Slope/y-intercept correction	Values after applying the slope/y-intercept correction.

Further information on the values **Slope**, **y-intercept**, **Bias correction** and **Slope/y-intercept correction**: *(see "Slope/y-intercept correction – Definition", chapter 5.13.2.6, page 1124)*

Further information on the value **SEP**: *(see "Figures of merit – Definition", chapter 5.13.1.19, page 1103)*

See also

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Slope/y-intercept correction – Definition (chapter 5.13.2.6, page 1124)

Slope/y-intercept correction – Tab (chapter 5.13.2.7, page 1126)

Slope/y-intercept corrections – Subsection (chapter 5.13.2, page 1117)

5.13.2.6 Slope/y-intercept correction – Definition

If a quantification model creates a systematic error during the prediction of samples with a known reference value, then a Slope/y-intercept correction can be created for this quantification model to correct this error.

Slope/y-intercept corrections can be selected in **PREDICT** commands to correct predicted results. In this case, the Slope/y-intercept correction can be used either during the determination run for samples that have not yet been measured or during the reprediction for samples that have already been measured.

To repredict predicted results, slope/y-intercept corrections can be selected in **Samples** ▶ **Results** ▶ **Predictions** ▶ **Reprocessing**.

The slope/y-intercept corrections are created and managed in **Models** ▶ **Slope/y-intercept corrections**.

The type of correction must be determined when the slope/y-intercept correction is created. The options **Bias** and **Slope/y-intercept** are available.

Bias correction

During bias correction, the average deviation between the reference value and the calculated value is corrected. The bias value is defined as:

$$\text{bias} = \bar{e} = \frac{1}{n}\sum_{i=1}^{n} e_i$$

Where *i* corresponds to a specific sample, $\bar{e}$ stands for the average deviation between reference value and calculated value, n represents the number of samples and e_i symbolizes the error of the samples.

A bias value of 0 indicates that the deviations are distributed randomly. A high bias value (positive or negative) indicates that a systematic error exists, such as adjustments or exchange of the instrument, the quality of the sample or the system.

Slope/y-intercept correction

During slope/y-intercept corrections, the slope and the y-intercept are corrected.

$$\text{slope} = b = \frac{s_{\hat{y}y}}{s_{\hat{y}}^2}$$

Where $s_{\hat{y}}^2$ corresponds to the covariance between the reference value and the calculated value and $s_{\hat{y}}^2$ stands for the variance of the n calculated values.

$$\text{intercept} = a = \bar{y} - b\bar{\hat{y}}$$

Where ***intercept*** stands for the y-intercept, $\bar{\hat{y}}$ corresponds to the mean value of the calculated values and $\bar{y}$ represents the mean value of the reference values.

See also

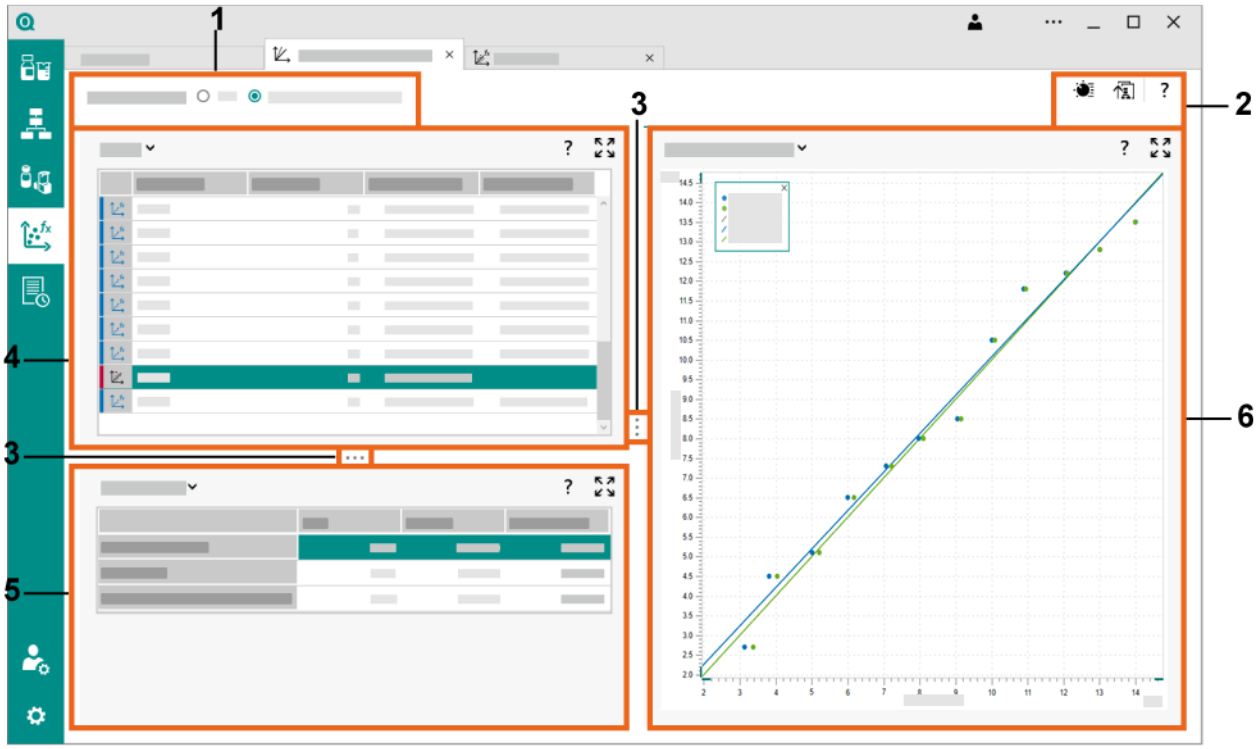
Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Models – Definition (chapter 5.13.1.1, page 1056)

Reprocessing predictions (chapter 5.10.13.5.1, page 363)

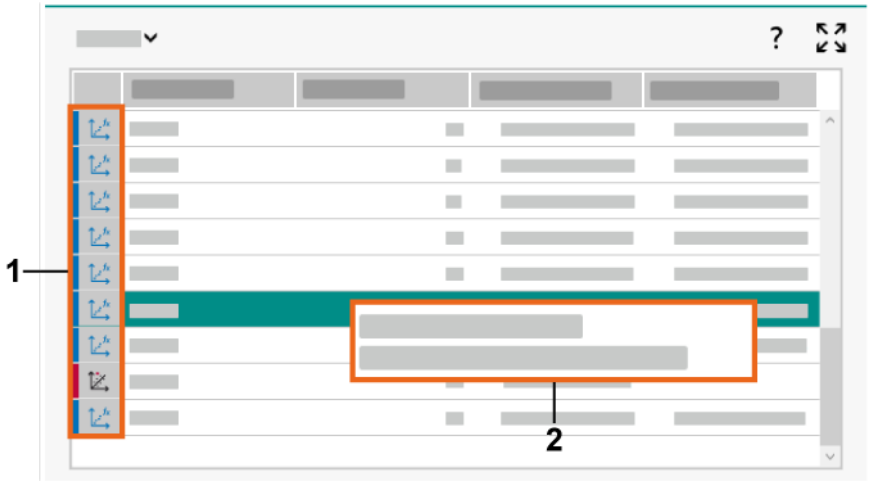
Slope/y-intercept correction – Tab (chapter 5.13.2.7, page 1126)

5.13.2.7 Slope/y-intercept correction – Tab



1	**Type of correction** Selection from the options **Bias** and **Slope/y-intercept**. Further information on the type of correction: *(see "Slope/y-intercept correction – Definition", chapter 5.13.2.6, page 1124)*	**2**	**Toolbar** Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*
3	**Divider** The size of the individual areas can be adjusted with the divider.	**4**	**Samples** Shows the samples whose data is used for the calculation of the slope/y-intercept correction. See detailed image *Samples*
5	**Correction values** Shows the **SEP**, **Slope**, and **y-intercept** values (calculated y-intercept coefficient) without correction, with bias correction and with slope/y-intercept correction, respectively. *(see "Calculations – Definition", chapter 5.10.13.1, page 348)*	**6**	**Correlation plot** Shows the correlation of the reference value and the predicted or corrected value. Further information on the correlation plot: *(see "Correlation plot – Area", chapter 5.13.1.20, page 1108)*

Samples



1 **Dataset display**
Shows whether the sample is included in the calculation or whether it is marked as an outlier.

2 **Context menu**
The context menu can be used to highlight a sample as an outlier.

See also

Correlation plot – Area (chapter 5.13.1.20, page 1108)

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Models – Definition (chapter 5.13.1.1, page 1056)

Slope/y-intercept correction – Definition (chapter 5.13.2.6, page 1124)

5.13.3 Identification models – Subsection

The following functions are available in **Models ▶ Identification models**:

- **Create identification model** creates a new identification model. Identification models can be developed, validated and published for use in the determination.
- Use **Import identification model** to import an OPMO file (**O**MNIS **P**rediction **Mo**del) as an identification model. Imported identification models can be edited and used, depending on their types.
- Use **Export identification model** to export the selected identification models as OPMO files (**O**MNIS **P**rediction **Mo**del).

-
  Reports for the selected identification models are generated with **Generate report**. The reports can be saved as a PDF file or also printed out.
-
  Use **Duplicate identification model** to duplicate the selected identification models under the same name and with a consecutive number.
-
  Use **Properties** to open the properties of the selected identification model.
-
  Use **Delete identification models** to delete the selected identification models and all identification models published from them. Samples and subsamples contained in the identification models are retained in the database.

Overview list

The following information is displayed in the overview list:

Name	Name of the identification model.
Version	Current version number of the identification model. A new version is created automatically with each saving process.
Type	Type of the identification model: ▪ **full** ▪ **light**
Last published version	Name and version number of the last published identification model.
Saved	Time at which the identification model was last saved.

If an **Identification model type light** is imported into the OMNIS Software for which there is no **Identification model type full** in the overview list, then **light** is displayed in the **Type** column.

See also

Creating identification model (chapter 5.13.3.4, page 1139)

Exporting a model (chapter 5.13.1.9, page 1079)

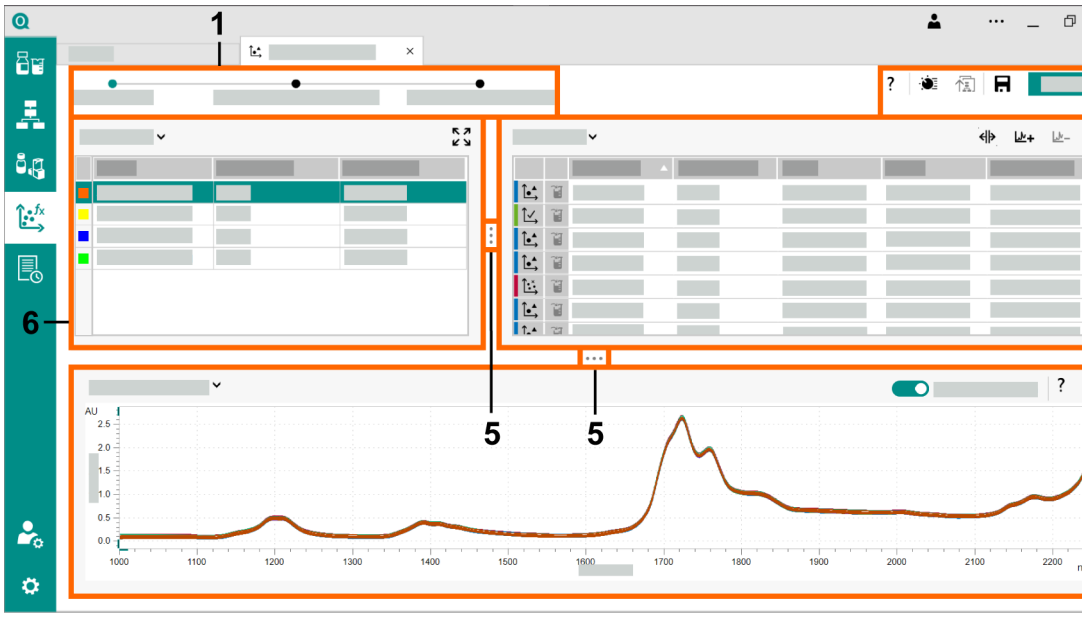
Importing models (chapter 5.13.1.8, page 1077)

Models – Definition (chapter 5.13.1.1, page 1056)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

5.13.3.1 Identification model – Tab

"Select samples" process step



1 Navigator

Selection from the **Select samples**, **Parameterize identification model** and **Validate identification model** process steps.

If incorrect entries have been made in the individual areas, then the respective process steps are displayed in **red**. By default, the process steps are displayed in **black** and the current selection in **green**.

2 Toolbar

Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

3 Spectra list

Displays spectra that are used in the identification model. See detailed image *Spectra list*.

Selecting a spectrum in the list causes that spectrum to be highlighted in the spectra overlay.

4 Spectra overlay

Shows the raw spectra from the spectra list overlaid. *(see "Spectra overlay – Area", chapter 5.13.1.16, page 1099)*

Selecting a spectrum in the Spectra overlay causes that spectrum to be highlighted in the spectra list.

The product colors of the spectra defined in the **product list** can be enabled by clicking on the toggle switch. Additional information on product colors: *(see "Product list – Area", chapter 5.13.3.6, page 1150)*

5 Divider

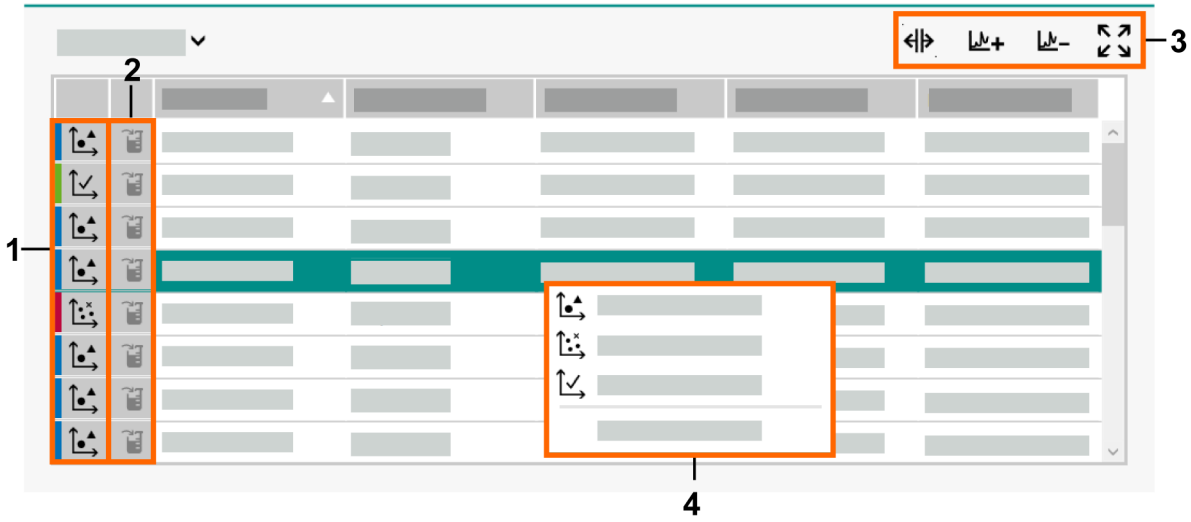
The size of the individual areas can be adjusted with the divider.

6 Product list

Displays products and product groups that are used in the identification model.

Selecting a product or several products in the product list displays the associated spectra in the spectra list and in the spectra overlay. A product can be renamed, merged with another product and assigned to a product group. Separate identification models can be created from product groups. *(see "Product list – Area", chapter 5.13.3.6, page 1150)*

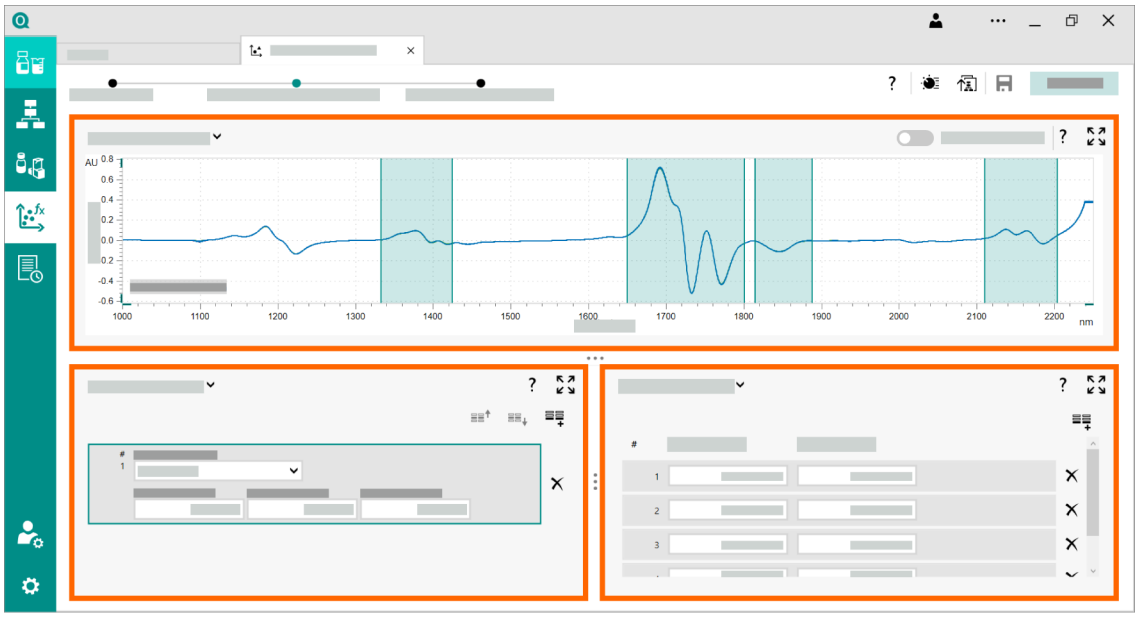
Spectra list



1	**Dataset display** Shows the dataset to which the spectrum belongs.	**2**	**Availability of the subsample in the database** Shows if the subsample is available in the database or if the spectrum has been imported from an external file.
3	**Toolbar** Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*	**4**	**Context menu** With the context menu, a spectrum can be assigned to a dataset or to a product.

"Parameterize the identification model" process step

The **Spectra overlay**, **Wavelength range** and **Data preprocessing** areas can be displayed in any area marked in orange:



- **Spectra overlay**
  Shows the preprocessed spectra from the spectra list overlaid.

  In the spectra overlay, the spectra are listed according to the filtering in the product list. *(see "Spectra overlay – Area", chapter 5.13.1.16, page 1099)*

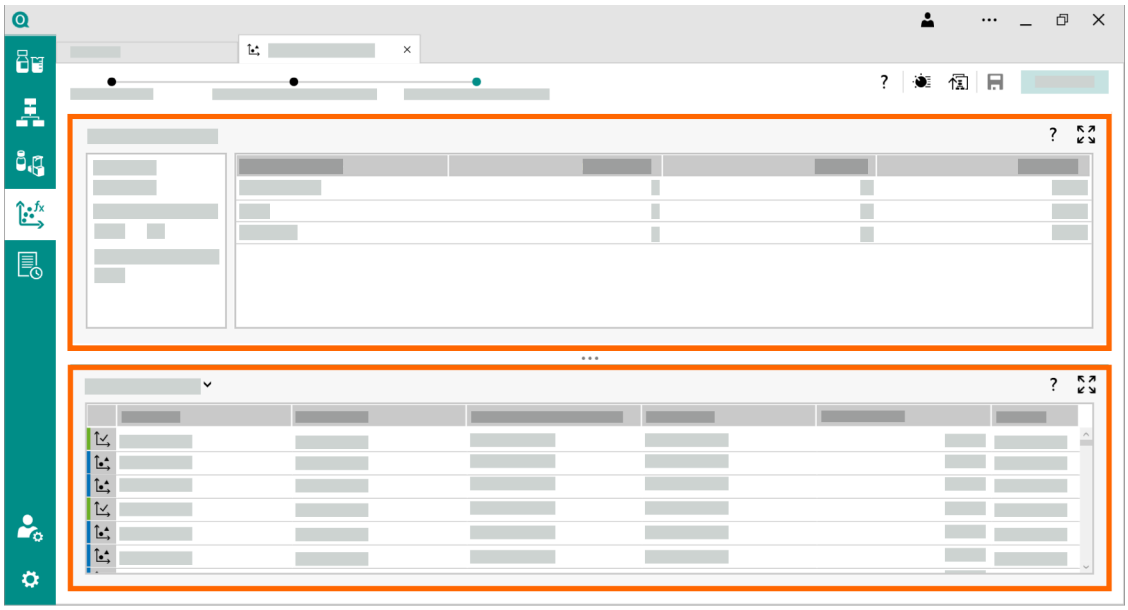
  The product colors defined in the **Select samples** process step can be enabled by clicking on the toggle switch. Additional information on product colors: *(see "Product list – Area", chapter 5.13.3.6, page 1150)*

- **Wavelength range**
  The desired wavelength range of the spectra overlay can be selected. *(see "Wavelength range – Area", chapter 5.13.1.18, page 1102)*

- **Data preprocessing**
  The required procedures for the data preprocessing of spectra can be selected and their order can be determined. *(see "Data preprocessing – Area", chapter 5.13.1.17, page 1100)*

"Validate identification model" process step

The **Validation overview** and **Validation results** areas can be displayed in any area marked in orange:



- **Validation overview**
  The number of successful and failed identifications of the samples is displayed in the 2 overviews (window and table). *(see "Validation overview – Area", chapter 5.13.3.7, page 1151)*

  Selecting a product in the list displays the spectra of the selected product in the **Validation results** area.

- **Validation results**
  Represents the evaluation of the spectra based on the model created and the probability that the sample is the identified product or the identified product group. *(see "Validation results – Area", chapter 5.13.3.8, page 1152)*

See also

Copying table (chapter 5.2.8, page 172)

Creating identification model (chapter 5.13.3.4, page 1139)

Editing identification model (chapter 5.13.3.5, page 1141)

Models – Definition (chapter 5.13.1.1, page 1056)

Product list – Area (chapter 5.13.3.6, page 1150)

Validation overview – Area (chapter 5.13.3.7, page 1151)

Validation results – Area (chapter 5.13.3.8, page 1152)

5.13.3.2 Identification model – Properties

Clicking on under **Models** ▶ **Identification models** opens the **Properties** window. The following information on the selected identification model is available in the **General** subsection:

General

Identification model	
Name	Name of the identification model.
Object ID	Identification number of the identification model.
Version	Version number of the identification model. A new version is created automatically each time an identification model is saved.
Created	Time at which the identification model was created.
Created by	User ID of the user who created the identification model.
Saved	Time at which the identification model was last changed.
Saved by	User ID of the user who changed the identification model.

Last published version	
Name	Name of the last published version of the identification model.
Object ID	Identification number of the last published version of the identification model.
Saved	Time at which the last published version of the identification model was saved.
Saved by	User ID of the user who last published the identification model.

Clicking on under **Models** ▶ **Identification models** within an opened identification model opens the **Properties** window. In the 2 subsections **General** and **Parameters**, the following functions and information are available:

General

Name	Name of the identification model (can be edited, max. 255 characters).
Object ID	Identification number of the identification model.
Version	Version number of the identification model. A new version is created automatically each time an identification model is saved.

Created	Time at which the identification model was created.
Created by	User ID of the user who created the identification model.
Saved	Time at which the identification model was last changed.
Saved by	User ID of the user who changed the identification model.

Parameters

Probability threshold	The probability threshold specifies the minimum probability that an analyzed spectrum for a product or product group needs to have in order to be assigned to that product or product group.

See also

Audit Trail – Directory (chapter 5.14.5, page 1177)

Creating identification model (chapter 5.13.3.4, page 1139)

Editing identification model (chapter 5.13.3.5, page 1141)

Identification model – Tab (chapter 5.13.3.1, page 1129)

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

Publishing models (chapter 5.13.1.11, page 1080)

5.13.3.3 Preparing identification model

These instructions describe 2 options how reference values can be entered before, during or after the measurement of the product information.

Alternatively, samples with already defined products can be imported from the XDS instrument or the DS instrument into the identification model. Additional information on importing spectra and their product information: *(see "Importing spectra and reference parameters", chapter 5.13.1.14.1, page 1098)*

- *Entering known product information manually*
- *Entering product information with the REQUEST command*

Entering known products manually

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Creating operating procedure with method

- Create a new method in **Processes** ▶ **Methods**.
- Click on to insert a **MEAS SPEC** command in the method. Parameterize the command in such a way that it acquires spectra of the samples. *(see "MEAS SPEC – Properties", chapter 5.11.8.31, page 674)*
- Assign the method to an operating procedure.

2 Creating sample profile

- In **Samples** ▶ **Sample profiles**, click on .
- Enter the desired name in the **Name of the sample profile** field.

3 Defining product parameters

Only one input field of the **Product** type can be added per sample profile.

- In the **Sample data** area, add another input field by clicking on .
- Enter the name of the product parameter in the **Field name short** field.
- Select the **Text** option in the **Type of input field** field.
  - Select the **Product** option in the **Use as** field.
  - Enable the **Editable field** check box so that a product can be added to the individual samples in the sample list.

or

- Select the **List elements** option in the **Type of input field** field.
  - Select the **Product** option in the **Use as** field.
  - In **List elements**, enter the desired list element.
- Enable the **Allow empty field** check box so that the **Default value** field can be left empty.
- Enable the **Force entry** check box so that the entry of a product is to forced for empty fields before the determination is started.
- In the **Operating procedures / subsamples** area, select the created operating procedure and enter the number "1" in **Number of subsamples**.
- Save the sample profile by clicking on .

4 Editing sample list

- In **Samples** ▶ **Sample lists**, create a new sample list or open an existing sample list.
- Select the sample profile and add the required number of samples to the sample list by clicking on .
- Add the created operating procedure to the subsamples.
- Enter the real reference values of the available product information under the reference values.
- Save the sample list by clicking on .
- Carry out the determination of the subsamples.

Entering products with the REQUEST command

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Creating sample profile

- In **Samples** ▶ **Sample profiles**, click on .
- Enter the desired name in the **Name of the sample profile** field.

2 Defining product parameters

Only one input field of the **Product** type can be added per sample profile.

- In the **Sample data** area, add another input field by clicking on .
- Enter the name of the product parameter in the **Field name short** field.
- Select the **Text** option in the **Type of input field** field.
- Select the **Product** option in the **Use as** field.
- Enable the **Editable field** check box so that a product can be added to the individual samples in the sample list.
- Enable the **Allow empty field** check box so that the **Default value** field can be left empty.
- Save the sample profile by clicking on .

3 Creating operating procedure with method

- Create a new method in **Processes** ▶ **Methods**.
- Click on to insert a **REQUEST** command in the method. Parameterize the command in such a way that it writes to the sample data. *(see "REQUEST – Parameters", chapter 5.11.8.77, page 794)*
- Click on to insert a **MEAS SPEC** command in the method. Parameterize the command in such a way that it acquires spectra of the samples. *(see "MEAS SPEC – Properties", chapter 5.11.8.31, page 674)*
- Assign the method to an operating procedure.

4 Assigning operating procedures to the sample profile

- Open the created sample profile in **Samples** ▶ **Sample profiles**.
- In the **Operating procedures / subsamples** area, select the created operating procedure.
- Under **Number of subsamples**, enter the number "1".

5 Entering products

- In **Samples** ▶ **Sample lists**, create a new sample list or open an existing sample list.
- Select the sample profile and add the required number of samples to the sample list by clicking on .
- Save the sample list by clicking on .
- Carry out the determination of the subsamples.
- During the determination of the sample, enter the reference values in the corresponding fields in an opened sample list under **Curves and data** ▶ **Live data**.

See also

Creating and deleting sample lists (chapter 5.10.1.1, page 211)

Creating and editing a method (chapter 5.11.3.3, page 418)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Creating and editing sample profile (chapter 5.10.5.2, page 261)

Creating quantification model (chapter 5.13.1.7, page 1074)

Importing spectra and reference parameters (chapter 5.13.1.14.1, page 1098)

MEAS SPEC – Properties (chapter 5.11.8.31, page 674)

REQUEST – Parameters (chapter 5.11.8.77, page 794)

Starting determination (chapter 5.10.8.6, page 304)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.3.4 Creating identification model

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Creating new identification model

- In **Models** ▶ **Identification models**, click on .

2 Entering name

- Enter the desired name in the **Name of the identification model** field.

The name can be changed at any time in the opened identification model in **Properties** ▶ **General**.

3 Selecting spectra

- Add the spectra either from the Sample lists or the Search queries of the OMNIS Software or import them from an XDS instrument or a DS instrument.

  Add spectra from sample lists or search queries of the OMNIS Software

  – Display all the sample lists saved in the database by clicking on **Sample lists**.
  or
  – Display all the search queries saved in the database by clicking on **Search queries**.
  – Select sample lists or search queries from which spectra are added to the identification model.
  All products and the corresponding number of spectra in the selected sample lists or search queries are displayed in the table on the right.

  or

  Importing spectra from XDS or DS instruments

  – To import spectra that were acquired with an XDS or DS instrument, click on **XDS/DS import**.
  – Click on .
  – Select the spectra files (.da) that are to be imported. The name of the spectra file determines the name of the product that is assigned to the added spectra.
  Note: If the previous selection of spectrum files is not to be overwritten, then disable the **Reset previously selected files** check box.
  – Click **[Open]** to confirm the selection.

No more than 1,000 spectra should be added to the identification model because such a high number of spectra can lead to an impairment of software performance.

4 Creating identification model

- Create the new identification model by clicking on **[Create]**.

5 Saving identification model

- Save the identification model by clicking on .

6 Editing identification model

- Edit the identification model, i.e. go through the process steps of the navigator and adjust the data as required.
  Instructions for editing identification models: *(see "Editing identification model", chapter 5.13.3.5, page 1141)*

See also

Copying table (chapter 5.2.8, page 172)

Editing identification model (chapter 5.13.3.5, page 1141)

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

Publishing models (chapter 5.13.1.11, page 1080)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.3.5 Editing identification model

An identification model is edited in 3 steps:

- *Select samples*
- *Parameterize identification model*
- *Validate identification model*

The following **prerequisites** must be fulfilled for all 3 steps:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The identification model is created: *(see "Creating quantification model", chapter 5.13.1.7, page 1074)*

Selecting samples

Prerequisite:

- The **Models** ▶ **Identification models** subsection is opened.
- An identification model is open and at the front. The navigator is in the **Select samples** process step.

Additional information on the navigator: *(see "Identification model – Tab", chapter 5.13.3.1, page 1129)*

1 Adding spectra (optional)

Selecting spectra

- Click on **+** in the **Spectra list** area.
- Add the spectra either from the Sample lists or the Search queries of the OMNIS Software. Spectra can also be imported from an XDS instrument or a DS instrument.

  Add spectra from sample lists or search queries
  - Display all the sample lists saved in the database by clicking on **Sample lists**.
    or
  - Display all the search queries saved in the database by clicking on **Search queries**.
  - Select sample lists or search queries from which spectra are added to the identification model.
    All products and the corresponding number of spectra in the selected sample lists or search queries are displayed in the table on the right.
  - Click on **[Add]** to confirm the selection.

  or

  Importing spectra from XDS or DS instruments
  - To import spectra that were acquired with an XDS or DS instrument, click on **XDS/DS import**.
  - Click on .
  - Select the spectra files (.da) that are to be imported. The name of the spectra file determines the name of the product that is assigned to the added spectra.
    Note: If the previous selection of spectrum files is not to be overwritten, then disable the **Reset previously selected files** check box.
  - Click **[Open]** to confirm the selection.

  No more than 1,000 spectra should be added to the identification model because such a high number of spectra can lead to an impairment of software performance.

- Add spectra by clicking on **[Add]**.

2 Deleting spectra (optional)

- To delete spectra from the spectra list, select the spectra and click on **–**.
  or
- Select spectra and delete using the **[DELETE]** key.

Note: The spectra are permanently deleted from the identification model. Imported spectra are also deleted in the OMNIS Software. Spectra measured in the OMNIS Software are retained in the database.

3 Renaming or merging products (optional)

- All products of the available spectra of the identification model are displayed in the **Product list** area.

All associated spectra are displayed by clicking on one or more products in the **Spectra list** and **Spectra overlay** areas.

- To change the product name, double-click on the required product in the **Product list** area.
- Enter the required name or select from the selection list.

Merging products

- To merge products, double-click on the required product in the **Product list** area.
- Enter an existing product name or select one from the selection list.
- In the next dialog, click on **[Merge]** to merge products with the same name.

Product groups can be assigned if, after validation of the identification model, the identification produces unsuccessful or ambiguous results. Additional information in the **Assign product group** step under *Validate identification model*.
Additional information on product groups: *(see "Product list – Area", chapter 5.13.3.6, page 1150)*

The identification model must contain at least 2 products or product groups.

4 Assigning a new or existing product (optional)

- In the **Spectra list** area, select all spectra for which a different product is to be assigned.
- Right-click on the selected spectra and select **Assign product** in the context menu.
- In the **New product** field, enter a new or an existing product name or select one from the selection list.
- Assign the new product to the selected spectra by clicking on **[Assign]**.

5 Deleting products and associated spectra (optional)

- Select all products to be deleted from the identification model in the **Product list** area.

- Right-click on the selected products and select **Delete selected products** in the context menu.
  or
- Use the **[DELETE]** key to delete the selected products.

Note: The products and the associated spectra are permanently deleted from the identification model. Imported spectra are also deleted in the OMNIS Software. Spectra measured in the OMNIS Software are retained in the database.

6 Determining and enabling product colors (optional)

Product colors are disabled by default and the colors of the datasets are used.
Additional information on color coding: *(see "Spectra overlay – Area", chapter 5.13.1.16, page 1099)*

- Click on the product color in the **Product list** area to open the color selector and select the desired color.
- In the **Spectra overlay** area, click on the **Display product colors** toggle switch to enable the product colors.

7 Splitting dataset automatically or manually

Splitting spectra list automatically

- In **Select samples** ▶ **Spectra list**, click on .
- Enable the toggle switch **Detect outliers** to automatically assign spectra to the outlier dataset and to define the significance level.
  Additional information on the significance level:
- Enable the **Determine validation dataset** toggle switch and define the percentage of spectra to be used for the validation dataset in the **Percentage** field.

- The following options can be enabled before the splitting of the dataset:
  - **Apply parameterization**: Applies the data preprocessings selected in the **Parameterize identification model** process step and the defined wavelength ranges to the spectra before the dataset is determined.
  - **Keep outliers**: The already existing outliers are retained and not taken into account in the split. This option can lead to an increase in the size of the outlier dataset, even if the significance level is not changed.
  - **Keep validation dataset**: The existing validation dataset is retained and not taken into account in the split. This option leads to an increase in the size of the validation dataset, even if the percentage of the validation dataset is not changed.
- Click on **[Split]** to confirm.
- If necessary, manually reprocess the automatically split spectra list.

or

Splitting spectra list manually

- Right-click on one or more spectra to open the context menu and assign the spectrum to the **Calibration dataset**, **Outlier dataset** or **Validation dataset**.

In order for the identification model to be calculated, at least 3 spectra must be assigned to the calibration dataset of each product or each product group.

As soon as at least one spectrum is selected in the spectra list, the spectrum is highlighted in the **Spectra overlay** area.

Parameterizing the identification model

Prerequisite:

- The **Models** ▶ **Identification models** subsection is opened.
- An identification model is open and at the front.
- All actions in the **Select samples** process step have been executed.

1 Change to the "Parameterize the identification model" process step

- In the navigator, change to the next process step of editing the identification model by clicking on **Parameterize identification model**.

The **Spectra overlay**, **Data preprocessing** and **Wavelength range** areas are available.

2 Adding data preprocessing

- Add data preprocessings under **Parameterize identification model** ▶ **Data preprocessing** by clicking on . By clicking on and , lines can be moved up or down and thus the order of application can be set.
- In the **Data preprocessing** field, select the type of data preprocessing and fill in the associated fields.

Additional information on the different data preprocessing methods and their parameters: *(see "Data preprocessing – Area", chapter 5.13.1.17, page 1100)*

The preprocessed spectra are shown immediately in the **Spectra overlay** area.

3 Defining the wavelength range

- Add wavelength ranges in **Parameterize identification model** ▶ **Wavelength range** by clicking on .
- Set the wavelength range manually or by using the **Spectra overlay** range:
  Defining wavelength range manually
  - Define the start wavelength in the **Start wavelength** column for each wavelength range.
  - Define the end wavelength in the **End wavelength** column for each wavelength range.
    or

  Set the wavelength range using the **Spectra overlay** area.
  - Click on the desired wavelength range in the **Wavelength range** area.
  - Click on **[Activate moving]** in the **Spectra overlay** area.
  - Move the cursor to the left edge of the highlighted area until the cursor is displayed as .
  - Hold down the left mouse button and move the left edge as desired.
  - Proceed in the same way on the right side of the highlighted area.
  - To move a wavelength range, move the cursor over the area until the cursor is displayed as ⇔. Hold down the left mouse button and move the area as desired.

- The wavelength ranges may not overlap.
- A minimum difference of 5 nm between start wavelength and end wavelength must be observed.

When defining the wavelength range in the **Spectra overlay** area, the values in the fields of the **Wavelength range** area are automatically adjusted.

The definition of the start wavelengths and end wavelengths is immediately displayed in the **Spectra overlay** area.

4 Calculating the identification model

- Calculate the identification model by clicking on **[Calculate]**.

For large spectra lists, this step may take some time.

If the **[Calculate]** button is disabled, then the following causes may apply:

- The identification model has already been calculated and has not been changed since then.
- An incorrect entry was made in one of the process steps. The process step of the affected area is displayed in **red** in the navigator. The field with the incorrect entry is outlined in red.
- An invalid value of the Probability threshold is entered under **Properties** ▶ **Parameters**.

Validating the identification model

Prerequisite:

- The **Models** ▶ **Identification models** subsection is opened.
- An identification model is open and at the front.
- All actions were executed in the **Select samples** and **Parameterize identification model** process steps.
- The identification model was calculated.

1 Change to the "Validate identification model" process step

- In the navigator, change to the next process step of editing the identification model by clicking on **Validate identification model**.

The **Validation overview** and **Validation results** areas are available.

2 Validating the identification model

- Check the results of the identification model in the **Validation overview** and **Validation results** areas.
  - In the **Validation overview** area, the number of failed and successful identifications for all spectra of the expected product or product group is displayed.
  - The identification results for the individual spectra of the associated product or product group are displayed in the **Validation results** area. Only the spectra of the calibration data set and the validation data set are validated.
  - In the **Validation overview** area, select the expected products or product groups to display detailed information on the spectra of the selected product or product group in the **Validation results** area.

Additional information on the validation overview: *(see "Validation overview – Area", chapter 5.13.3.7, page 1151)*
Additional information on the validation results: *(see "Validation results – Area", chapter 5.13.3.8, page 1152)*

3 Editing the identification model again or adjusting the probability threshold (optional)

- If the identification model needs to be optimized after checking the validation results, then the identification model settings can be adjusted in the previous process steps.
- The Probability threshold can also be edited.
  Execute the following steps to adjust the Probability threshold:
  - Open the properties of the identification model by clicking on .
  - Select **Parameters** in the selection list.
  - Adjust the value of the **Probability threshold**.
  - Recalculate the identification model and check the results.

Additional information on the Probability threshold: *(see "Identification model – Properties", chapter 5.13.3.2, page 1133)*

4 Assigning a product group (optional)

Product groups can be defined if the identification produces ambiguous results despite changed Probability threshold and settings of the model.

In this case, all products that have the same ambiguous results are each assigned to a product group. In the identification of the spectra, these product groups are treated as individual identifiable products.

To define the product group:

- Switch to the **Select samples** process step in the navigator.
- Double-click on the required input field in the **Product list** area in the **Product group** column.
- Enter the name of the product group or select it from the selection list.
- Recalculate the identification model.

The identification model must contain at least 2 products or product groups.

5 Creating an identification model from a product group (optional)

If the identification produces ambiguous results, separate identification models can be created from selected product groups.

To create an identification model from the product group:

- Select at least one product group under **Select samples** ▶ **Product list** or under **Validate identification model** ▶ **Validation overview**. If several product groups are selected, then an identification model is created for each product group.
- Right-click on the selected product group to open the context menu and select **Create identification models from product groups**. The number of selected product groups is displayed in the context menu.

An identification model of the selected product group is opened in a new tab. The defined datasets, data preprocessing and wavelength ranges are applied to the newly created identification model. The product group is not applied in the newly created identification model.

6 Saving identification model

- Save the identification model by clicking on .

The version and the change date of the identification model are updated automatically in **Properties** ▶ **General**.

7 Publishing identification model

- Instructions for publishing identification models: *(see "Nearest Neighbor Distance – Definition", chapter 5.13.1.10, page 1080), (see "Publishing models", chapter 5.13.1.11, page 1080)*

The identification model must be published in order to enable its use in determinations or in model hierarchies.

See also

Creating identification model (chapter 5.13.3.4, page 1139)

Importing spectra and reference parameters (chapter 5.13.1.14.1, page 1098)

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

Publishing models (chapter 5.13.1.11, page 1080)

Sample list – Tab (chapter 5.2.2, page 159)

User rights – Directory (chapter 4.5.7.4, page 89)

5.13.3.6 Product list – Area

The defined products, the corresponding number of spectra and the product groups are displayed as a table in the **Product list** area. The **Product list** is used in the following subsection:

- Under **Models** ▶ **Identification models** in the **Select samples** process step.

As soon as one or more products are highlighted in the **Product list** area, the associated spectra will be displayed in the **Spectra list** area. A product can be renamed, merged with another product, assigned to a product group, and deleted from the identification model. Separate identification models can be created from product groups.

Additional information on renaming, merging, assigning, and deleting products in the identification model: *(see "Editing identification model", chapter 5.13.3.5, page 1141)*
Additional information on creating identification models from product groups: *(see "Editing identification model", chapter 5.13.3.5, page 1141)*

Each product in the **Product list** area is automatically assigned a product colour. The product color can be changed manually by clicking on the colored square. If there are more products than available colors, then the colors are repeated.

Additional information on color coding: *(see "Spectra overlay – Area", chapter 5.13.1.16, page 1099)*

Additional information on the activation of product colors: *(see "Identification model – Tab", chapter 5.13.3.1, page 1129)*

Additional information on the spectra overlay area: *(see "Spectra overlay – Area", chapter 5.13.1.16, page 1099)*

The following information is displayed in the product list:

Product	Name of the product defined in the sample list or product list.
Number of spectra	The number of spectra that are assigned to the product.
Product group	Name of the product group assigned to the product.

See also

Creating identification model (chapter 5.13.3.4, page 1139)

Models – Definition (chapter 5.13.1.1, page 1056)

5.13.3.7 Validation overview – Area

The results of the identification are displayed in the **Validation overview** area. The **Validation overview** area is used in the following subsections:

- Under **Models** ▶ **Identification models** in the **Validate identification model** process step
- Under **Models** ▶ **Model hierarchies** in the **Validate model hierarchy** process step

Under **Identification models** and **Model hierarchies**, the **Validation overview** area is subdivided into 2 overviews, 1 window on left side and 1 table on the right side. The window shows a summary of all spectra in the model or model hierarchy. The table shows the results of the individual products or product groups.

Only identification models are taken into account when validating model hierarchies.

Quantification models are checked for existence only in the database.

Windows

Successful %	Number of successful identifications in percent.
Successful	Number of successful identifications.
Failed	Number of failed identifications.

Number of spectra	Total number of all spectra.

Table

Product / product group (only identification model)	Name of the (expected) product or (expected) product group. **Note**: Further identification models can be created from product groups. Additional information: *(see "Editing identification model", chapter 5.13.3.5, page 1141)*
Product (only model hierarchy)	Name of the product. **Note**: The top line **Total** shows the total number of identifications.
Failed	Number of failed identifications. The identification is considered to have failed if the expected product does not match the identified product or if the expected product group does not match the identified product group. **Notice**: Ambiguous results are also considered to have failed.
Successful	Number of successful identifications. The identification is considered successful if it matches the expected product or product group.
Successful %	Number of successful identifications in percent.

See also

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Creating identification model (chapter 5.13.3.4, page 1139)

Editing identification model (chapter 5.13.3.5, page 1141)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

Models – Definition (chapter 5.13.1.1, page 1056)

Validation results – Area (chapter 5.13.3.8, page 1152)

5.13.3.8 Validation results – Area

The identification results of the spectra from the calibration dataset and the validation dataset are listed in the **Validation results** area. The **Validation results** are displayed in the following subsections:

- Under **Models** ▶ **Identification models** in the **Validate identification model** process step

- Under **Models** ▶ **Model hierarchies** in the **Validate model hierarchy** process step

The contents in the **Validation results** area depend on the selection or the marking of the products or product groups in the **Validation overview** area. This means that only the identifications that are selected in the table of the **Validation overview** area are displayed. Multiple products or product groups can be selected at the same time.

- *Identification model table*
- *Model hierarchy table*

Identification model

	The spectrum is assigned to the calibration dataset.
	The spectrum is assigned to the validation dataset.
Sample name	Name of the sample.
Subsample name	Name of the subsample.
Expected product / product group	Name of the expected product or expected product group.
Probability	The type of result is decisive for the results displayed. 3 possibilities can be presented here: ▪ **Probability of successful identification**: In this case, the probability with which the spectrum was assigned to the expected product or product group is displayed. ▪ **Probability of ambiguous identification**: In this case, all probabilities of the products or product groups that were able to be assigned to the spectrum are displayed one below the other. The probability with which the spectrum was assigned to the expected product or the expected product group always comes first. Below this, the remaining results are displayed in descending order of probability. ▪ **Probability of failed identification**: In this case, the probability corresponding to the expected product or product group is displayed.

Identified as	▪ If the identification is successful, the name of the identified product or product group is displayed, which matches the name of the expected product or product group. ▪ If the identification fails, then the status of the identification will be displayed: **Unidentified** or **Ambiguous**.
Validation result	Result of the validation. Possible results: ▪ **Successful**: The expected product or product group corresponds to the result of the identification. ▪ **Failed**: No identification or ambiguous identification. The expected product or product group does not correspond to the result of the identification.

Model hierarchy

Only identification models are taken into account when validating model hierarchies.

Quantification models are checked for existence only in the database.

	The spectrum is assigned to the calibration dataset.
	The spectrum is assigned to the validation dataset.
Sample information ▪ **Sample name** ▪ **Subsample name** ▪ **Expected product**	The following information is grouped under Sample information: ▪ Name of the sample. ▪ Name of the subsample. ▪ Name of the expected product.

Model hierarchy result ▪ **Identified as** ▪ **Validation result**	The following information is grouped under Model hierarchy result: ▪ If the identification is successful, the name of the identified product is displayed. If the identification fails, then the status of the identification is displayed, i.e. it is specified in greater detail why unambiguous identification is not possible: **Unidentified** or **Ambiguous**. ▪ Result of the validation. Possible results: – **Successful**: The expected product corresponds to the result of the identification. – **Failed**: No identification or ambiguous identification. The expected product does not correspond to the result of the identification.
Result Level [n] ▪ **Identified as** ▪ **Status**	The following information is grouped under result level [n]: ▪ Name of the product identified at the respective level. ▪ Status of the identification at the respective level: **Identified**, **Unidentified** or **Ambiguous**.

See also

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Creating identification model (chapter 5.13.3.4, page 1139)

Editing identification model (chapter 5.13.3.5, page 1141)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

Models – Definition (chapter 5.13.1.1, page 1056)

Validation overview – Area (chapter 5.13.3.7, page 1151)

5.13.4 Model hierarchy – Definition

A model hierarchy is a nested model in which different submodels are used according to the result. Model hierarchies are used to make more precise predictions when the informative value of a single model is insufficient. When creating and developing models, it can happen that the spectra of two or more products are so similar that they cannot be sufficiently distinguished from each other, even with the help of parameterization. The products that cannot be unambiguously identified are defined as a product group in the main model, for which a new submodel can then be created. This submodel can be linked to its respective product group in the model hierarchy editor using drag and drop to create a model hierarchy.

Once the informative value of linking several identification models is sufficient, additional quantification models can be added to the model hierarchy. Quantification models extend the model hierarchy to include quantitative parameters of interest. To correct systematic errors in quantification models within the model hierarchy, slope/y-axis intercept corrections can be assigned if required.

Additional information on creating a model hierarchy:
(see "Creating and editing a model hierarchy", chapter 5.13.4.3, page 1161)
Additional information on parameters of interest:
(see "Models – Definition", chapter 5.13.1.1, page 1056)

Model hierarchies are created and managed under **Models** ▶ **Model hierarchies**. A published model hierarchy can be selected instead of a single model in PREDICT commands in order to evaluate spectra.

All models and spectra are retained when a model hierarchy is deleted. Only the links between the models are lost.

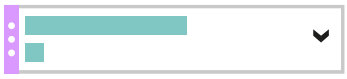
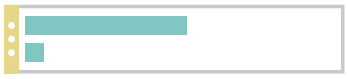
Depiction

Models are represented as blocks within a model hierarchy. These blocks contain the name and the current version number of the model. Products contain only the name.

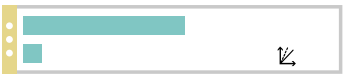
Model hierarchies distinguish between 2 types of collapsible and expandable symbols:

- A vertical arrow shows that this identification model contains products and/or product groups. The main model is always open by default.
- A horizontal arrow shows that a submodel is linked to this product group.

Color coding distinguishes between the following elements:

- 
  Identification model
- 
  Quantification model
-
  Product or product group

In addition to this color coding, symbols are used to provide additional information on the respective elements:

- 

  Quantification model with slope/y-intercept correction

-

  An element under this path is faulty. All linked elements of this path have this symbol.

There is no graphical distinction between a product and a product group in the model hierarchy editor. The type of the element is defined in the respective identification model.

See also

Creating a slope/y-intercept correction (chapter 5.13.2.3, page 1120)

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Editing identification model (chapter 5.13.3.5, page 1141)

Editing quantification model (chapter 5.13.1.12, page 1082)

Model hierarchy – Tab (chapter 5.13.4.2, page 1159)

Models – Definition (chapter 5.13.1.1, page 1056)

Nearest Neighbor Distance – Definition (chapter 5.13.1.10, page 1080)

Publishing models (chapter 5.13.1.11, page 1080)

5.13.4.1 Model hierarchies – Subsection

The following functions are available under **Models** ▶ **Model hierarchies**:

-

  With **Create model hierarchy**, a new model hierarchy is created and then the model hierarchy editor is opened. Model hierarchies can be created, edited and published for use in the determination.

-

  With **Import model hierarchy**, an OPMO file (**O**MNIS **P**rediction **Mo**del) is imported as a model hierarchy. The models and products it contains are part of the OPMO file and are also imported. Imported model hierarchies can be edited and used, depending on their type.

-

  With **Export model hierarchies**, the selected model hierarchies are exported as OPMO files (**O**MNIS **P**rediction **Mo**del). The models and products it contains are part of the OPMO files and are also exported.

-

  Generate report is used to generate reports for the selected model hierarchies. The reports can be saved as a PDF file or also printed out.

-

  The properties of the selected model hierarchy are opened with **Properties**.
-

  With **Delete model hierarchies**, the selected model hierarchies and all model hierarchies published from them are deleted. Models contained in the model hierarchies are retained in the database.

Overview list

The following information is displayed in the overview list:

Name	Name of the model hierarchy.
Version	Current version number of the model hierarchy.
Type	Type of the model hierarchy: ▪ **full** ▪ **light**
Last published version	Name and version number of the last published model hierarchy.
Saved	Time at which the model hierarchy was last saved.

If a Model hierarchy type light is imported into the OMNIS Software for which there is no Model hierarchy type full in the overview list, then **light** is displayed in the **Type** column.

See also

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Exporting model hierarchies (chapter 5.13.4.6, page 1168)

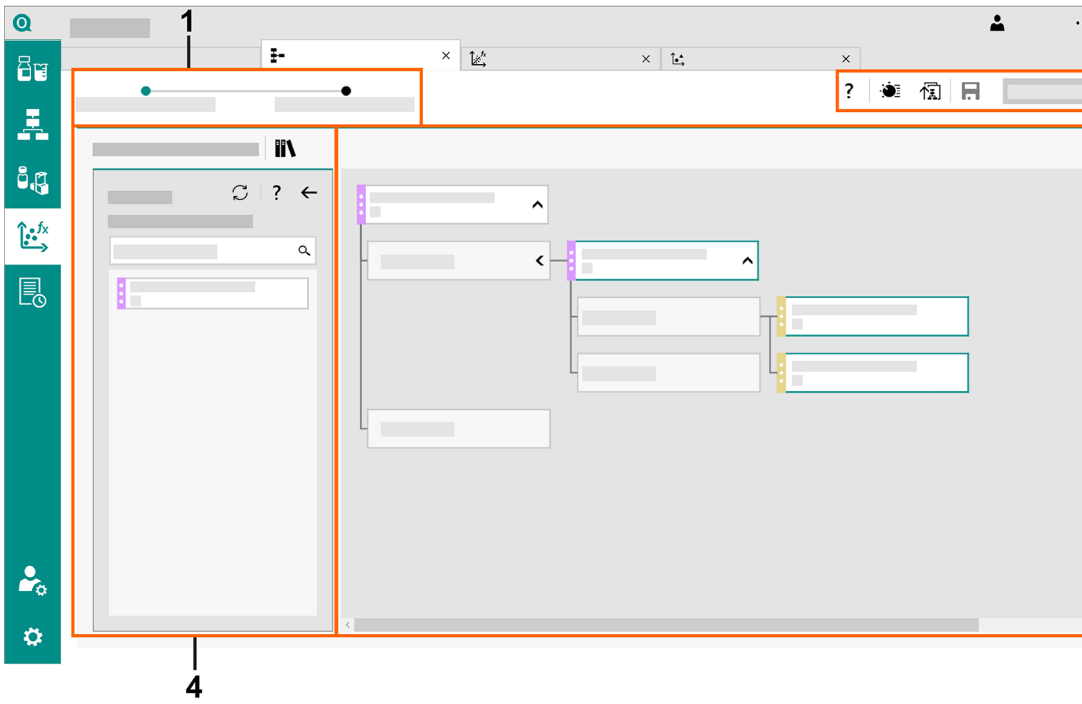
Importing a model hierarchy (chapter 5.13.4.5, page 1167)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

5.13.4.2 Model hierarchy – Tab

"Editing the model hierarchy" process step



1 Navigator
Selection from the **Edit model hierarchy** and **Validate model hierarchy** process steps.

2 Toolbar
Validate, save and publish a model hierarchy.

Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

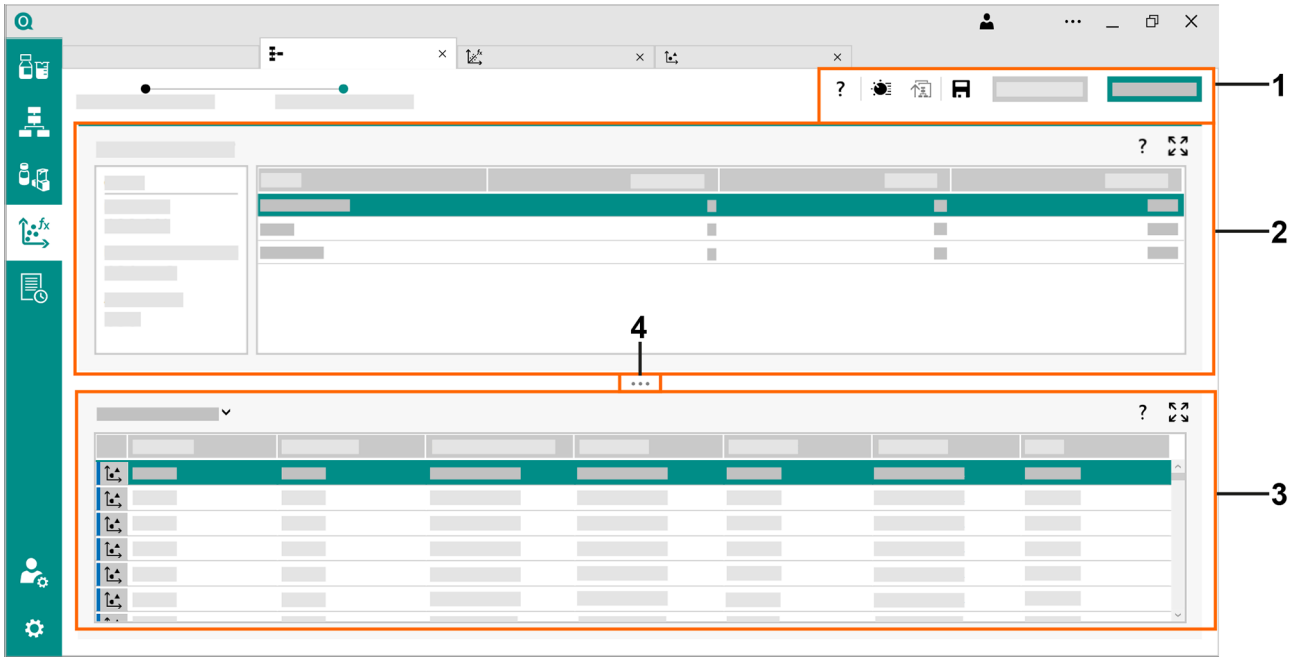
3 Model hierarchy editor
Model hierarchies can be created and edited using drag and drop with the model hierarchy editor. Additional models can be added from the **Model library**.

Additional information on creating and editing model hierarchies: *(see "Creating and editing a model hierarchy", chapter 5.13.4.3, page 1161)*

4 Model library
Shows a list of models that can be added to the model hierarchy.

Additional information on libraries: *(see "Library – Brief description", chapter 5.2.1, page 157)*

"Validating a model hierarchy" process step



1 Toolbar

Validate, save and publish a model hierarchy.

Additional information on the functions of the individual icons: *(see "OMNIS Software – Overview of functions", chapter 5.3, page 173)*

2 Validation overview

The results of the validation are shown in the 2 overviews in the **Validation overview** area.

Additional information on the validation overview: *(see "Validation overview – Area", chapter 5.13.3.7, page 1151)*

3 Validation results

The validated spectra are listed in the **Validation results** area.

Additional information on the validation results: *(see "Validation results – Area", chapter 5.13.3.8, page 1152)*

4 Divider

The size of the individual areas can be adjusted with the divider.

See also

Copying table (chapter 5.2.8, page 172)

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

5.13.4.3 Creating and editing a model hierarchy

A model hierarchy is created and edited in 2 steps:

- *Create and edit model hierarchy*
- *Validate model hierarchy*

The following **prerequisites** must be fulfilled for both steps:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

Creating and editing a model hierarchy

Prerequisite:

- The **Model** ▶ **Model hierarchies** subsection is opened.
- A new model hierarchy is created by clicking on or an existing model hierarchy is edited by double-clicking.
- The **Edit model hierarchy** process step is selected.

Additional information on the navigator: *(see "Model hierarchy – Tab", chapter 5.13.4.2, page 1159)*

1 Naming or renaming a model hierarchy

- Open the **Properties** window by clicking on in the top toolbar.
- Enter the desired name in the **Name** field under **Properties** ▶ **General**.

The following characters are not allowed: **. | ' " { }**

2 Adding the main model

Selecting a main model

- Click on to open the **Library** window.
- Under **Library** ▶ **Identification models**. use drag and drop to insert the identification model into the model hierarchy editor.

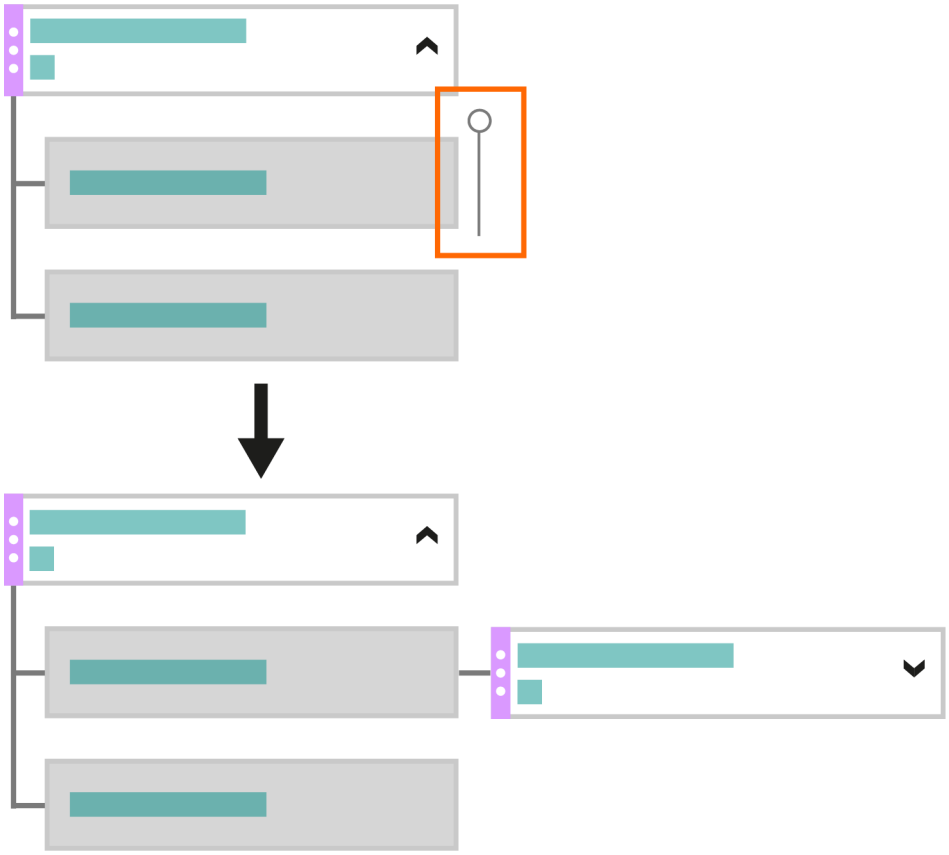
Additional information on libraries: *(see "Library – Brief description", chapter 5.2.1, page 157)*

3 Linking models with product groups or products

Selecting the models

There is no graphical distinction between a product and a product group in the model hierarchy editor. The type of the respective element is defined in the identification model.

- Click on to open the **Library** window. Click on to reload the list of displayed models.
- Models are edited in the model hierarchy editor using drag and drop. By clicking and holding the mouse button on the desired model under **Library** ▶ **Identification models** or **Library** ▶ **Quantification models**, the model can be moved to the model hierarchy editor and linked to other models, products or product groups. A green vertical line next to a product group shows the insertion position for a model.
  - Only one Identification model can be linked to a product or product group at a time.
  - Any number of Quantification models can be linked to a product or a product group.



The following options are available for inserting and editing models:

- Models within the model hierarchy can be removed from the model hierarchy by clicking on .
- The properties of a selected model, product or product group can be opened by clicking on .
- Submodels cannot be moved within a model hierarchy once they have been linked. The corresponding submodel can be deleted and linked again, if required.
- Models cannot be edited in the model hierarchy editor. The model must be opened in the corresponding subsection for editing.

4 Adding the slope/y-intercept correction to the quantification model (optional)

- Select the quantification model in the model hierarchy editor to which a slope/y-intercept correction is assigned.
- Open the properties of the selected quantification model by clicking on .
- Assign the desired slope/y-intercept correction under **Properties** ► **Parameters**.

5 Saving and publishing the model hierarchy

- Save the model hierarchy by clicking on .
- Publish the model hierarchy by clicking on .

Model hierarchies can be published without validation. The validation process compares the expected products with the identified products and checks the links within the model hierarchy for errors. Metrohm recommends successfully completing the validation process.

Validating a model hierarchy (optional)

Prerequisite:

- The **Models** ► **Model hierarchies** subsection is opened.

- All actions in the **Edit model hierarchy** process step have been executed.

1 Changing to the "Validate model hierarchy" process step

- In the navigator, click on **Validate model hierarchy** to switch tor the next process step.

The **Validation overview** and **Validation results** areas are available.

2 Validating the model hierarchy internally or externally

Only identification models are taken into account when validating model hierarchies.

Quantification models are checked for existence only in the database.

Validate internally

Click on the **Validate internally** to compare the expected products with the identified products and check the links within the hierarchy for errors.

Only the spectra of the main model are used for internal validation.

Validating externally

- Click on **Validate externally** to select spectra from sample lists, search queries or import for validation.

- Add the spectra either from the Sample lists or the Search queries of the OMNIS Software or import them from an XDS instrument or a DS instrument.

  Selecting spectra from sample lists or search queries

  – Display all the sample lists saved in the database by clicking on **Sample lists**.

    or

  – Display all the search queries saved in the database by clicking on **Search queries**.
  – Select sample lists or search queries from which spectra are selected for validation.

    Depending on the selected sample lists or search queries, the **Product / number of spectra** list shows different entries.
  – Click on **[Validate]** to confirm the selection.

  or

  Importing spectra from XDS or DS instruments

  – To import spectra that were acquired with an XDS or DS instrument, click on **XDS/DS import**.
  – Click on .
  – Select the spectra file (.da) that is to be imported.
  – Click **[Open]** to confirm the selection.
  – Click on **[Validate]**.

The results of the validation are displayed in the **Validate model hierarchy** process step. If the external validation is repeated with other data, then the existing data is replaced.

Additional information on the validation overview: *(see "Validation overview – Area", chapter 5.13.3.7, page 1151)*

Additional information on validation results: *(see "Validation results – Area", chapter 5.13.3.8, page 1152)*

See also

Model hierarchies – Subsection (chapter 5.13.4.1, page 1157)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

Model hierarchy – Properties (chapter 5.13.4.4, page 1166)

Model hierarchy – Tab (chapter 5.13.4.2, page 1159)

Models – Definition (chapter 5.13.1.1, page 1056)

5.13.4.4 Model hierarchy – Properties

Clicking on under **Models** ▶ **Model hierarchies** opens the **Properties** window. The following information on the selected model hierarchy is available in the **General** subsection:

General

Model hierarchy	
Name	Name of the model hierarchy.
Object ID	Identification number of the model hierarchy.
Version	Version number of the model hierarchy. A new version is created automatically each time a model hierarchy is saved.
Created	Time at which the model hierarchy was created.
Created by	User ID of the user who created the model hierarchy.
Saved	Time at which the model hierarchy was last saved.
Saved by	User ID of the user who last saved the model hierarchy.

Last published version	
Name	Name of the last published version of the model hierarchy.
Object ID	Identifier of the last published version of the model hierarchy.
Saved	Time at which the last published version of the model hierarchy was saved.
Saved by	User ID of the user who last published the model hierarchy.

Clicking on under **Models** ▶ **Model hierarchies** within an opened model hierarchy in the **Edit model hierarchy** process step opens the **Properties** window. The following information for the selected element is available in the **General** subsection:

General

Identification model	
Name	Name of the identification model.
Object ID	Identification number of the identification model.

Identification model	
Version	Version number of the identification model. A new version is created automatically each time an identification model is saved.

Quantification model	
Name	Name of the quantification model.
Object ID	Identification number of the quantification model.
Version	Version number of the quantification model. A new version is created automatically each time a quantification model is saved.

Product / product group	
Name	Name of the product or product group.

Click on under **Models** ▶ **Model hierarchies** to open the **Properties** window within an opened model hierarchy in the **Edit model hierarchy** process step. A slope/y-intercept correction for the selected quantification model can be assigned in the **Parameters** subsection:

Parameters

Quantification model	
Slope/y-intercept correction	Name of the slope/y-intercept correction.

See also

Model hierarchy – Definition (chapter 5.13.4, page 1155)

Models – Definition (chapter 5.13.1.1, page 1056)

5.13.4.5 Importing a model hierarchy

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

- At least one OMNIS model file (**.opmo**) of a model hierarchy is available.

1 Selecting model hierarchy

- Click on to open the **Import a model hierarchy** window in **Models** ▶ **Model hierarchies**.

2 Browsing for folder

- Select the folder in which the desired model hierarchy is saved.

3 Selecting file

- Select the OMNIS model file or enter the name of the OMNIS model file in the **File name** field.

4 Confirming and importing selection

- Click **[Open]** to confirm the selection.

The model hierarchy is imported into the OMNIS Software.

- If the model hierarchy is already available in the database, then it can either be overwritten or created as a new version.
- The models and slope/y-axis intercept corrections contained in the model hierarchy are also imported. If an element already exists in the database, then it will be skipped during import.

See also

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Exporting model hierarchies (chapter 5.13.4.6, page 1168)

5.13.4.6 Exporting model hierarchies

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- At least one model hierarchy is available in the overview list.

1 Selecting model hierarchies

- Select the desired model hierarchies under **Models** ▶ **Model hierarchies**.
- Open the **Export model hierarchies** window by clicking on .

2 Selecting the export type

- Select the **Export type** from the selection list.
  - **Model hierarchy type light**
  - **Model hierarchy type full**

Only model hierarchies of the same type can be exported at the same time. Additional information on the export types **Type full** and **Type light**: *(see "Model hierarchy – Definition", chapter 5.13.4, page 1155)*

3 Selecting or entering a target folder

- Select the target folder by clicking on or enter the absolute path in the address bar.

4 Creating OMNIS model hierarchy files

- Export the OMNIS model hierarchy files (OPMO files) into the target folder by clicking on **[Export]**. One or more OPMO files are exported under the respective name of the model hierarchies.
- Click on **[Open target folder]** to open the target folder.

The models and slope/y-axis intercept corrections contained in the model hierarchy are also exported.

All time indications are converted into Coordinated Universal Time (UTC±00:00) when exporting. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.

The local time on the computer is used for the date and time displayed in the file name.

See also

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Importing a model hierarchy (chapter 5.13.4.5, page 1167)

Model hierarchy – Definition (chapter 5.13.4, page 1155)

5.13.4.7 Publishing model hierarchy

To use a model hierarchy for determinations, it must be published. This means that the model hierarchy can still be developed further without impacting the published version – and thus the determinations.

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The model hierarchy to be published has been saved.

Validation is optional for model hierarchies for publishing. Additional information on validating model hierarchies: *(see "Creating and editing a model hierarchy", chapter 5.13.4.3, page 1161)*

1 Opening model hierarchy

- In **Models** ▶ **Model hierarchies**, open the desired model hierarchy.

2 Opening dialog

- Open the **Publish model hierarchy** dialog by clicking on .

3 Updating methods (optional)

- To update methods that use this model hierarchy, enable the **Update methods** check box.

This option only applies if an existing and already used model hierarchy was changed and is published again. Signed and published methods will not be changed. If the filtering of the data permissions is enabled, then only methods with the data permissions of the currently logged-in user will be updated.
Additional information on data permissions: *(see "Data permissions – Definition", chapter 4.5.9, page 105)*

4 Publishing model

- Publish the model hierarchy by clicking on **[Publish]**.

The last published version of the model hierarchy is displayed in the overview list and is available for the determination in the parameters of the **PREDICT** command.

Additional information on using model hierarchies in the determination: *(see "PREDICT – Parameters", chapter 5.11.8.16, page 610)*

If a published model hierarchy used in a method is deleted, the method cannot be executed anymore.

See also

Creating and editing a model hierarchy (chapter 5.13.4.3, page 1161)

Exporting model hierarchies (chapter 5.13.4.6, page 1168)

Importing a model hierarchy (chapter 5.13.4.5, page 1167)

PREDICT – Parameters (chapter 5.11.8.16, page 610)

User rights – Directory (chapter 4.5.7.4, page 89)

5.14 Audit Trail – Actions

The following actions can be executed in the **Audit Trail** work area:

-
  Audit Trail entries are exported, archived and checked for integrity under **Audit TrailSearch queries**. Search queries can be created and saved to filter Audit Trail entries. A report can be generated for data on Audit Trail entries that correspond to the currently applied filter criteria of the Audit Trail search query.

Information on the Audit Trail in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

See also

Archiving Audit Trail (chapter 5.14.9, page 1192)

Audit Trail – Directory (chapter 5.14.5, page 1177)

Audit Trail – Status (chapter 5.14.7, page 1186)

Checking Audit Trail integrity (chapter 5.14.4, page 1176)

Creating report (chapter 5.10.1.4, page 224)

Displaying and managing the process overview (chapter 5.14.3.1, page 1174)

Exporting Audit Trail (chapter 5.14.8, page 1187)

Filtering Audit Trail - Search queries (chapter 5.14.6, page 1184)

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Process overview – Definition (chapter 5.14.3, page 1173)

User management (Active Directory) – Actions (chapter 4.4, page 41)

User management (OMNIS) – Actions (chapter 4.5, page 43)

User rights – Directory (chapter 4.5.7.4, page 89)

5.14.1 Audit Trail search queries – Subsection

The following functions are available under **Audit Trail** ► **Audit Trail-Search queries**:

-
  With **Create Audit Trail search query**, a new Audit Trail search query is created in which Audit Trail entries can be searched for using filter criteria. The results can be saved as an Audit Trail search query for later use.
-
  Delete Audit Trail search query deletes the selected Audit Trail search query. The Audit Trail entries contained therein are retained in the database.

Overview list

The following information is displayed in the overview list:

Name	Name of the Audit Trail search query. The name can be adjusted after opening the Audit Trail search query.
Saved	Time at which the Audit Trail search query was last saved.

See also

Audit Trail – Directory (chapter 5.14.5, page 1177)

Creating and editing Audit Trail - Search queries (chapter 5.14.2, page 1172)

Filtering Audit Trail - Search queries (chapter 5.14.6, page 1184)

5.14.2 Creating and editing Audit Trail-Search queries

Creating and editing Audit Trail search queries

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

- The **Audit Trail** work area is open.

1 Creating or editing an Audit Trail search query

- Click on .
  or
- Click on an existing Audit Trail search query.

A new tab with an empty Audit Trail search query is opened.

2 Naming Audit Trail search query

- Enter the desired name in the name field and confirm it with **[Enter]**.

3 Configuring filter criteria

- Open the filter and define the required filter criteria by clicking on .

Additional information on filtering search queries and server search queries: *(see "Filtering Audit Trail - Search queries", chapter 5.14.6, page 1184)*

4 Saving an Audit Trail search query

- Save the search query by clicking on .
  or
  Click on and select the **Save as new search query** option to save the configured filter criteria as a new search query.

The name entered is displayed on the tab.

See also

Filtering Audit Trail - Search queries (chapter 5.14.6, page 1184)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Search queries – Definition (chapter 5.10.2, page 243)

User rights – Directory (chapter 4.5.7.4, page 89)

5.14.3 Process overview – Definition

The **process overview** is used to display the process sequence at the time of an action (create, insert, change, remove or delete) performed by the user on an **operating procedure** or **method**. This function enables the traceability of the processes.

The process overview is available for Audit Trail entries created with OMNIS Software version 3.0.0 or higher.

See also

Archiving Audit Trail (chapter 5.14.9, page 1192)

Audit Trail – Actions (chapter 5.14, page 1171)

Command – Properties (chapter 5.11.8.1, page 431)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Displaying and managing the process overview (chapter 5.14.3.1, page 1174)

Exporting Audit Trail (chapter 5.14.8, page 1187)

Method – Definition (chapter 5.11.3, page 413)

Methods – Subsection (chapter 5.11.3.1, page 414)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Processes – Actions (chapter 5.11, page 378)

5.14.3.1 Displaying and managing the process overview

Prerequisite:

- The user has performed an action (create, insert, change, remove or delete) on an operating procedure or method in the **Processes** work area.
- Audit Trail is activated.
- The **Audit Trail** work area is open.
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*

1 Selecting the Audit Trail entry

- Click on an entry for the **Operating procedure** or **Method** object type in the Audit Trail.

The detail view of the selected Audit Trail entry is updated.

The process overview is available for Audit Trail entries created with OMNIS Software version 3.0.0 or higher.

2 Displaying the process overview

- Open the dialog with the process overview in the **Detail view** by clicking on .

3 Opening and closing objects (optional)

- Objects with ❮■ contain additional commands and methods:
  - Display the commands and methods contained in the object by clicking on ❯.
  - Close the object by clicking on ❮.

4 Displaying object properties

- Display the object properties by clicking on an object in the process overview.

Additional information on object properties in the Audit Trail: *(see "Audit Trail – Directory", chapter 5.14.5, page 1177)*.

Zooming the chart with the mouse wheel

1 Positioning the cursor

- Position the cursor on the desired section.

2 Zooming in the chart

- Rotate the mouse wheel.
  - Rotate forward: Increase section horizontally and vertically.
  - Rotate backward: Reduce size of section horizontally and vertically.

The desired area is magnified or reduced.

3 Resetting the view

- Reset the process overview to the default view by clicking on **Reset view** at the bottom left of the dialog.

See also

Archiving Audit Trail (chapter 5.14.9, page 1192)

Audit Trail – Actions (chapter 5.14, page 1171)

Command – Properties (chapter 5.11.8.1, page 431)

Commands – Definition (chapter 5.11.8, page 429)

Creating and editing an operating procedure (chapter 5.11.1.3, page 387)

Exporting Audit Trail (chapter 5.14.8, page 1187)

Method – Definition (chapter 5.11.3, page 413)

Methods – Subsection (chapter 5.11.3.1, page 414)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Operating procedure – Definition (chapter 5.11.1, page 379)

Operating procedures – Subsection (chapter 5.11.1.1, page 380)

Process overview – Definition (chapter 5.14.3, page 1173)

5.14.4 Checking Audit Trail integrity

Information on the Audit Trail in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- User management is activated.
- Audit Trail is enabled.
- The **Audit Trail-Search queries** subsection in the **Audit Trail** work area is opened.

1 Opening integrity check

- Click on to open the **Check integrity** dialog.

2 Starting integrity check

- Click on **[Continue]** to start the integrity check.

This may take several minutes.

All Audit Trail entries are checked for completeness and integrity. Subsequently, a dialog opens with the result of the integrity check.

3 Exporting the report on the integrity errors

- Click on **[Export]** to export a report on the integrity errors found as a CSV file.

The integrity errors found are discarded when the dialog is closed. The integrity check must be repeated in order to find the integrity errors once again and subsequently export them.

In addition, 4 additional files are exported and saved in the target folder for the integrity check of the CSV file. The integrity of the CSV file can be checked either by executing the exported EXE file

(**CheckCSV.exe**) or alternatively by using OpenSSL. Instructions for both options are described in the exported TXT file (**Readme.txt**). An Audit Trail entry of the run is recorded.

To check the integrity of the exported CSV file, first ensure that no other CSV file is present in the target folder. The CSV file must be closed when the integrity check is executed. The integrity check of the CSV file can no longer be executed if the files created in this process are moved or deleted.

The integrity check is available with OMNIS Software version 3.0.0 or higher. The integrity of Audit Trail entries created prior to OMNIS Software version 3.0.0 is checked only with this OMNIS Software or higher. No integrity error will be found with the integrity check if these Audit Trail entries were corrupted or deleted before installation of OMNIS Software version 3.0.0.

See also

Archiving Audit Trail (chapter 5.14.9, page 1192)

Audit Trail – Actions (chapter 5.14, page 1171)

Exporting Audit Trail (chapter 5.14.8, page 1187)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

User rights – Directory (chapter 4.5.7.4, page 89)

5.14.5 Audit Trail – Directory

Click on ↻ to update the list in the Audit Trail.
Non-unique objects, e.g. functional units that can change, are displayed as N/A.

In the **OMNIS Client/Server system**, the Audit Trail can be used centrally on the OMNIS Server. For this, all the entries of all the connected OMNIS Clients from the entire **OMNIS Client/Server system** are displayed in the Audit Trail.
If the connection to the OMNIS Server is interrupted, only the local Audit Trail entries are displayed. Therefore, it must be noted that the entries may be incomplete in case of an interrupted connection.
Information on the Audit Trail in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Audit Trail

Level	Classification of the action. *(see "Audit Trail – Status", chapter 5.14.7, page 1186)*
Date/Time	Date and time of the action that was executed.
Category	Category that the action is assigned to.
Action	Brief description of the action, e.g.: ▪ Created ▪ Deleted ▪ Modified
Object type	Type of the object on which the action was carried out.
Object name	Name of the object.
Object ID	Unambiguous designation of the object.
User ID	Unambiguous designation of the user who is logged into the OMNIS Software or on an external client (e.g. instrument).
User name	Complete name of the user who is logged into the OMNIS Software or on an external client (e.g. instrument).
Transaction ID	Unambiguous designation of the transaction. If several entries can be linked to the same user action, the same transaction ID is used for all of them.
Client	Name of the computer or instrument on which the action was carried out. **Note**: In the **OMNIS Client/Server system** the unique name of the OMNIS Client that can be assigned only once in the entire **OMNIS Client/Server system**.

Object properties

Additional information is listed in the object properties. The first 7 entries are always entered in the list by default. The contents of the **Detail view** are adapted in accordance with the selected action. The following entries can be displayed in the object properties:

Object name	Name of the object.
Object type	Type of the object with which the action was carried out.
Object ID	Unambiguous designation of the object.

Action	Brief description of the action, e.g.: ▪ Created ▪ Deleted ▪ Modified
Transaction ID	Unambiguous designation of the transaction. If several entries can be linked to the same user action, the same transaction ID is used for all of them.
Client	Name of the computer in the network on which the action was carried out.
Operation mode	Operation mode in which the OMNIS Software is used.

Additional entries in the **Detail view**:

Activation mode	Type of the licensing process (e.g. offline licensing or online licensing).
Reason for modification	Selected reason for modification at the time of saving.
Modification comment	Optional comment on the change.
Connected to	Name of the functional unit to which the digital sensor, the OMNIS Liquid Adapter, the solution with bottle cap single-use or the solution with bottle cap multi-use is currently connected.
Operating procedure ID	Unambiguous designation of the operating procedure.
Operating procedure name	Name of operating procedure.
Article number	Number of the article.
Executed action	Action that was carried out by manual control of a functional unit.
Current database size	Current database size of the local database.
Command ID	Unambiguous designation of the command.
Command name	Name of the command.

Command type	Type of the command.
Reason	Reason for the failed user login.
User ID	Designation of the user for whom login to the OMNIS Software or on an external client has failed.
Computer name	Unique identifier used to locate the computer.
Computer name old	Computer name of the OMNIS Client that was replaced in the **OMNIS Client/Server system**. **Note**: Applicable only in the **OMNIS Client/Server system**.
Computer name new	Computer name of the OMNIS Client that was added to the **OMNIS Client/Server system** as a replacement. **Note**: Applicable only in the **OMNIS Client/Server system**.
File name	Name of the imported file or name of the backup of the database. Name and complete path in the Audit Trail export.
Directory	File directory in which the backup was placed.
Database version	Version of the database.
Decision	Decision (button) when confirming the message.
Result	Result of the integrity check.
Tag ID	Unambiguous designation of the memory chip in the label of the bottle cap.
Firmware version	Version number of the firmware.
Functional unit	Name of the Functional unit used within a command.
Instrument name	Name of instrument.
Overall status	Status of the wavelength test.
Host name	Name of the Cubis II Balance in the network.
Identification model	Name of the identification model.

Identification model ID	Unambiguous designation of the identification model type full.
Channel	Number of the measuring channel for which the reference standardization was executed.
Comment	Comment on the action.
License number	Number of the license (only applies to online licensing).
Last calibration on	Last calibration of the Cubis II Balance.
Message	Text of the message.
Message number	Six-digit number of the message.
Measuring mode	Measuring mode in which the reference standardization was executed.
Method ID	Unambiguous designation of the method.
Method name	Name of the method.
Method version	Version of the method.
Model hierarchy	Name of the model hierarchy.
Model hierarchy ID	Unambiguous designation of the model hierarchy type full.
New operation mode	Operation mode that is to be used for the OMNIS system.
OMNIS build version	Build version of the OMNIS Software.
Package version	Firmware version that is installed on the balance.
Placed on	Name of the sample robot where the sample rack is placed on its rack base.
Position	Number (e.g. RP7) of the rack position on the rack base of the sample robot.
Sample ID	Unambiguous designation of the sample.
Sample list name	Name of the sample list.
Sample name	Name of the sample.

Product batch	Product batch of the solution.
Product number	Number of the product.
Product type	Type of the product.
Program version	Version of the program.
Q-App version	Version of the Q-App on the balance with which the connection to the OMNIS Software was established.
Quantification model	Name of the quantification model.
Quantification model ID	Unambiguous designation of the quantification model type full.
Rack code	Rack code of the imported Sample Processor Rack.
Interface	Selection of the interface that was used to execute the reference standardization.
Sensor type	Type of the sensor.
Serial number	Serial number of the product.
Name of standard	Name of the reflection standard or transmission standard.
ID of standard	Unambiguous designation of the external reflection standard or transmission standard.
Type of standard	Type of the reflection standard or transmission standard.
Key	Manual control (press of a key) on a functional unit.
Subsample ID	Unambiguous designation of the subsample.
Subsample name	Name of the subsample.
Signature level	Level of the signature that was added or deleted.
Signature comment	Signature comment that was created at the time of signature.
Reason for signature	Reason that was selected when signing.
Version	Version of the object.

Certification date	Date on which the most recent certification of the standard was carried out.
Related object IDs	Listing of the unique designations of subsamples with reference to an Audit Trail entry.

Changed values

Old and new values are listed as Further information with the changed values. The contents under the modified values are adapted in accordance with the selected action.

Designation	Designation of the changed value.
Path	Designation of the source of the change: ▪ Method and command in which the changed value was created. ▪ Functional unit that was added, removed, replaced or on which values were changed.
Action	Brief description of the action, e.g.: ▪ Created ▪ Deleted ▪ Modified
Old value	Value prior to the change.
New value	Changed value after the saving process.

See also

Archiving Audit Trail (chapter 5.14.9, page 1192)

Audit Trail – Actions (chapter 5.14, page 1171)

Audit Trail – Status (chapter 5.14.7, page 1186)

Exporting Audit Trail (chapter 5.14.8, page 1187)

Filtering Audit Trail - Search queries (chapter 5.14.6, page 1184)

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Sorting the overview list (chapter 5.2.7, page 171)

User rights – Directory (chapter 4.5.7.4, page 89)

5.14.6 Filtering Audit Trail-Search queries

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- User management is activated.
- The Audit Trail is enabled.
- The **Audit Trail-Search queries** subsection in the **Audit Trail** work area is opened.

1 Opening Audit Trail search queries

- Open the **Audit Trail** ▶ **Audit Trail-Search queries** subsection.

2 Opening filter

- Open the filter by clicking on .

The area for selecting configurable filter criteria is opened.

3 Selecting logical connective

Select a logical connective from the selection list.

- **All filter criteria must be met**
  - Only search results matching all the selected filter criteria will be displayed in the list.
- **At least one filter criterion must be met**
  - Search results matching at least one filter criterion will be displayed in the list.

4 Adding filter criterion

- Add a filter criterion by clicking on .

Any number of filter criteria can be added to refine the search.

5 Selecting filter criterion

- Select a filter criterion from the selection list.

Depending on the filter criterion, a variety of search operators and options to choose from are available.

6 Defining filter criterion further

- Select a search operator from the selection list, if necessary:
  - **Contains**
    Finds the entries that contain the input in the defined filter criterion.
  - **Equals**
    Finds the entries for which the value in the defined filter criterion corresponds exactly with the input.
  - **Does not equal**
    Finds the entries for which the value in the defined filter criterion does not correspond with the input.
- Enter or select a search term, a number of days, a value or a date, depending on the filter criterion selected previously.
  If no selection list with search operators is displayed, the required value for the filter criterion can be entered directly.

7 Filtering

- Apply the selected filter criteria by clicking on **[Filter]**.

The results are displayed in the list according to the filter criteria.

8 Selecting page

- Click on ← or → to display the next or the previous page of the list.
- Click on ⇤ or ⇥ to display the first or the last page of the list.
- Alternatively, enter the page number directly in the input field and confirm with **[Enter]**.

The selected page is displayed.

The filter is reapplied when the pages are changed.

9 Resetting filter

- Reset changes to the filter criteria to the last status saved by clicking on **[Reset]**.

The results are displayed in the list according to the filter criteria.

10 Removing filter criterion

- Remove the filter criterion by clicking on ✕.

If a filter criterion is deleted, then the filter needs to be applied again to see the corresponding entries.

11 Closing filter

- Click on ▼ or ↑ to close the filter.

The filter criteria remain active, even after closing the filter.

The area for selecting configurable filter criteria is closed.

Information on the Audit Trail in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Audit Trail – Directory (chapter 5.14.5, page 1177)

Sorting the overview list (chapter 5.2.7, page 171)

User rights – Directory (chapter 4.5.7.4, page 89)

5.14.7 Audit Trail – Status

In the Audit Trail, you can filter according to a specific level*(see "Filtering Audit Trail - Search queries", chapter 5.14.6, page 1184)*.

In the overview list of the **Audit Trail** work area, the levels are shown as follows in the **Level** column:

Overview of the levels

⊗	**Error** An **Error** is shown as soon as an action has failed, e.g. in the case of a run error or an error during login or authentication.
⚠	**Warning** A **Warning** is shown when data or settings have been modified or deleted in the entire OMNIS Software, e.g. when modifying sample and subsample data after an analysis, evaluations and calculations, when archiving samples or the Audit Trail and with user actions in manual operation or in connection with status changes in the sample list. In addition to that, warnings are also documented during execution of a determination on this level.

Information

A **Information** is shown when non-critical actions are executed, e.g. when creating samples and sub-samples, during Audit Trail export, when a user logs into the OMNIS Software, when authenticating signatures and when connecting hardware.

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Filtering Audit Trail - Search queries (chapter 5.14.6, page 1184)

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Software – Overview of functions (chapter 5.3, page 173)

Sorting the overview list (chapter 5.2.7, page 171)

User rights – Directory (chapter 4.5.7.4, page 89)

5.14.8 Exporting Audit Trail

Instructions on exporting Audit Trail entries:

- *Export Audit Trail*

Instructions for improving the readability of the export file:

- *Displaying complete and legible entries in HTML format in Microsoft Excel*
- *Displaying the process overview*

Information on the Audit Trail in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Exporting Audit Trail

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- User management is activated.
- The Audit Trail is enabled.

- The **Audit Trail-Search queries** subsection in the **Audit Trail** work area is opened.

1 Applying filter criteria

- Click on to open the filter and select a logical connective from the selection list to define whether all or at least one of the defined filter criteria is to apply.

Only the Audit Trail entries that correspond to the currently applied filter criteria are displayed in the exported CSV file.

For more information regarding the filtering of entries in the Audit Trail, see: *(see "Filtering Audit Trail - Search queries", chapter 5.14.6, page 1184)*

2 Exporting Audit Trail

- Click on to open the window to enter the file name and the target folder.

3 Selecting or entering target folder

- Select the target folder or enter the absolute path in the address bar where the exported file is to be saved.

4 Defining file name

- Enter the name under which the file is to be saved in the **File name** field.

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

5 Creating file

- Create the CSV file by clicking on **[Save]**.

In addition, 4 additional files are exported and saved in the target folder for the integrity check of the CSV file. The integrity of the CSV file can be checked either by executing the exported EXE file (**CheckCSV.exe**) or alternatively by using OpenSSL. Instructions for both options are described in the exported TXT file (**Readme.txt**). An Audit Trail entry of the run is recorded.

This may take several minutes.
The file has the valid time stamp of the time at which the export was started by clicking on .

To check the integrity of the exported CSV file, first ensure that no other CSV file is present in the target folder. The CSV file must be closed when the integrity check is executed. The integrity check of the CSV file can no longer be executed if the files created in this process are moved or deleted.
Additional information on the integrity check in the Audit Trail: *(see "Checking Audit Trail integrity", chapter 5.14.4, page 1176)*

All time indications are converted into Coordinated Universal Time (UTC±00:00) when exporting. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.

Displaying complete and legible entries in HTML format in Microsoft Excel

Prerequisite:

- The export of the Audit Trail entries has been executed.

1 Opening CSV file

- Open the CSV file in a spreadsheet program (e.g. Microsoft Excel).

The OMNIS Software enables exporting large amounts of data. However, Microsoft Excel is not a default program for opening and displaying Audit Trail entries. To display large amounts of data in full in Microsoft Excel, the built-in data tool MS Power Query can be used.

2 Copying content

- Select a cell containing HTML data in the **Value** column and double-click to open it.
- Mark the entire content of the cell with the left mouse button.
- Display the context menu with the right mouse button and click on **[Copy]**.

3 Inserting content

- Add a new sheet.

- Right-click on a cell and select **[Paste Special]** in the context menu.
- Select **Unicode Text** in the dialog and paste the contents by clicking on **[OK]**. Then save the CSV file.

Information regarding the Audit Trail entries, e.g. the object type message, is displayed in its entirety and in legible format in the CSV file.

When highlighting the HTML data to be copied in the desired cell of the CSV file, only the contents of this cell may be highlighted. When highlighting the complete cell, the options described above are not displayed.

Displaying process overview

Prerequisite:

- The export of the Audit Trail entries has been executed.

1 Opening CSV file

- Open the CSV file in a spreadsheet program (e.g. Microsoft Excel).

2 Copying process overview

- In the desired line of object type **Operating procedure** or **Method** select the cell in the **Process overview** column.
- Display the context menu with the right mouse button and click on **[Copy]**.

3 Opening text editor

- Open a text editor (e.g. Notepad).

4 Inserting content

- Display the context menu with the right mouse button and click on **[Insert]**.

5 Reading the process overview

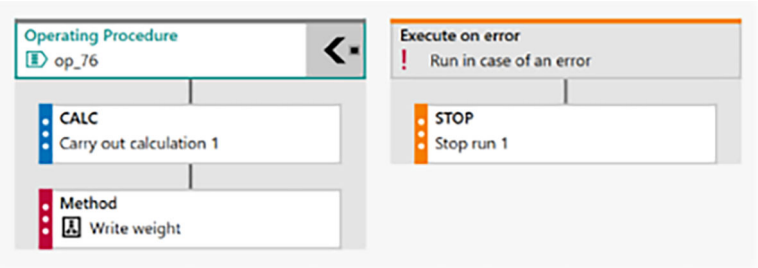
Observe the following rules when reading the exported process overview:

- The hierarchical structure between objects is represented by lines. The object at the beginning of a line (top) contains the objects at the end of the line (bottom).
- Optional sequences are displayed in the lower part of the exported process overview.

- The object type is automatically added in front of each object (e.g. **Wait 1** command is displayed as **Command Wait 1** and **Test** method as **Method Test**).

Example 1

Display of the process overview in the OMNIS Software:

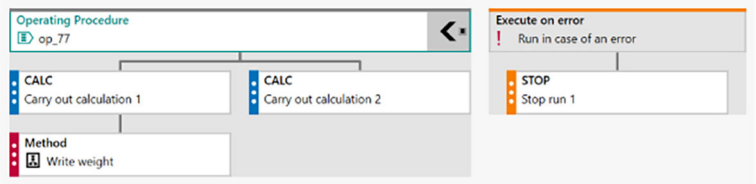


Display of the process overview in the file:

```
Operating procedure op_76
  ├─Command Carry out calculation 1
  ├─Method Write weight
  └─Run sequence Run in case of an error
     └─Command Stop run 1
```

Example 2

Display of the process overview in the OMNIS Software:



Display of the process overview in the file:

```
Operating procedure op_77
  │  │
  │  │  ├─Command Carry out calculation 1
  │  │  └─Method Write weight
  │  │
  │  │  └─Command Carry out calculation 2
  └─Run sequence Run in case of an error
     └─Command Stop run 1
```

See also

Archiving Audit Trail (chapter 5.14.9, page 1192)

Audit Trail – Actions (chapter 5.14, page 1171)

Displaying and managing the process overview (chapter 5.14.3.1, page 1174)

Exporting operating procedures and methods (chapter 5.11.1.5, page 393)

Exporting subsample data (chapter 5.10.1.3, page 220)

Filtering Audit Trail - Search queries (chapter 5.14.6, page 1184)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Process overview – Definition (chapter 5.14.3, page 1173)

User rights – Directory (chapter 4.5.7.4, page 89)

5.14.9 Archiving Audit Trail

Instructions on archiving Audit Trail entries:

- *Archiving the Audit Trail*

Instructions for improving the readability of the archive file:

- *Displaying complete and legible entries in HTML format in Microsoft Excel*
- *Displaying the process overview*

Archiving Audit Trail entries is possible only in **OMNIS Stand-Alone**.

Information on the Audit Trail in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Archiving Audit Trail

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- User management is activated.
- The Audit Trail is enabled.
- The **Audit Trail-Search queries** subsection in the **Audit Trail** work area is opened.

1 Archiving Audit Trail

- Start archiving by clicking on and continue the process by clicking on **[Archive]**.

A window is opened.

The currently used filter criteria are not applied when archiving.
All the Audit Trail entries are archived and deleted from the current database.

2 Entering file name

- Enter the name under which the file is to be saved in the **File name** field.

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

3 Selecting or entering target folder

- Select the target folder or enter the absolute path in the address bar in which the archived file is to be saved.

4 Creating archive file

- Create the CSV file by clicking on **[Save]**.

In addition, 4 additional files are exported and saved in the target folder for the integrity check of the CSV file. The integrity of the CSV file can be checked either by executing the exported EXE file (**CheckCSV.exe**) or alternatively by using OpenSSL. Instructions for both options are described in the exported TXT file (**Readme.txt**). All the Audit Trail entries are deleted from the current database and an Audit Trail entry for the process run is created.

This may take several minutes.
The archived file has the valid time stamp of the time at which the archiving was started by clicking on **[Save]**.

To check the integrity of the exported CSV file, first ensure that no other CSV file is present in the target folder. The CSV file must be closed when the integrity check is executed. The integrity check of the CSV file can no longer be executed if the files created in this process are moved or deleted.
Additional information on the integrity check in the Audit Trail:
(see "Checking Audit Trail integrity", chapter 5.14.4, page 1176)

All time indications are converted into Coordinated Universal Time (UTC±00:00) when archiving. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.

Displaying complete and legible entries in HTML format in Microsoft Excel

Prerequisite:

- The archiving of the Audit Trail entries has been executed.

1 Opening CSV file

- Open the CSV file in a spreadsheet program (e.g. Microsoft Excel).

The OMNIS Software enables archiving large amounts of data. However, Microsoft Excel is not a default program for opening and displaying Audit Trail entries. To display large amounts of data in full in Microsoft Excel, the built-in data tool MS Power Query can be used.

2 Copying content

- Select a cell containing HTML data in the **Value** column and double-click to open it.
- Mark the entire content of the cell with the left mouse button.
- Display the context menu with the right mouse button and click on **[Copy]**.

3 Inserting content

- Add a new sheet.
- Right-click on a cell and select **[Paste Special]** in the context menu.
- Select **Unicode Text** in the dialog and paste the contents by clicking on **[OK]**. Then save the CSV file.

Information regarding the Audit Trail entries, e.g. the object type message, is displayed in its entirety and in legible format in the CSV file.

When highlighting the HTML data to be copied in the desired cell of the CSV file, only the contents of this cell may be highlighted. When highlighting the complete cell, the options described above are not displayed.

Displaying process overview

Prerequisite:

- The archiving of the Audit Trail entries has been executed.

1 Opening CSV file

- Open the CSV file in a spreadsheet program (e.g. Microsoft Excel).

2 Copying process overview

- In the desired line of object type **Operating procedure** or **Method** select the cell in the **Process overview** column.
- Display the context menu with the right mouse button and click on **[Copy]**.

3 Opening text editor

- Open a text editor (e.g. Notepad).

4 Inserting content

- Display the context menu with the right mouse button and click on **[Insert]**.

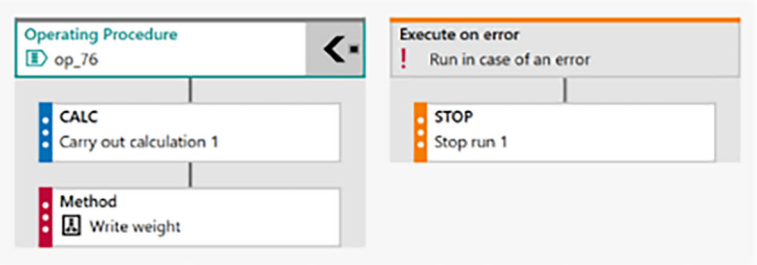
5 Reading the process overview

Observe the following rules when reading the archived process overview:

- The hierarchical structure between objects is represented by lines. The object at the beginning of a line (top) contains the objects at the end of the line (bottom).
- Optional sequences are displayed in the lower part of the archived process overview.
- The object type is automatically added in front of each object (e.g. **Wait 1** command is displayed as **Command Wait 1** and **Test** method as **Method Test**).

Example 1

Display of the process overview in the OMNIS Software:

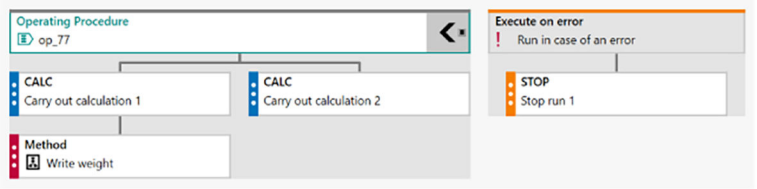


Display of the process overview in the file:

```
Operating procedure op_76
  ├─Command Carry out calculation 1
  ├─Method Write weight
  └─Run sequence Run in case of an error
     └─Command Stop run 1
```

Example 2

Display of the process overview in the OMNIS Software:



Display of the process overview in the file:

```
Operating procedure op_77
  │  │  ├─Command Carry out calculation 1
  │  │  └─Method Write weight
  │  └─Command Carry out calculation 2
  └─Run sequence Run in case of an error
     └─Command Stop run 1
```

See also

Audit Trail – Actions (chapter 5.14, page 1171)

Displaying and managing the process overview (chapter 5.14.3.1, page 1174)

Exporting Audit Trail (chapter 5.14.8, page 1187)

Filtering Audit Trail - Search queries (chapter 5.14.6, page 1184)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Process overview – Definition (chapter 5.14.3, page 1173)

User rights – Directory (chapter 4.5.7.4, page 89)

5.15 Settings – Actions

Information on the settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

You can execute the following actions in the subsections of the **Settings** work area:

-

  The dialog language is changed and the Include preliminary run test functions and the emergency stop function are enabled or disabled inn **Settings** ▶ **General settings**. A default printer can also be selected and the notification settings can be set.

-

  The system language is adapted and the User management (OMNIS) or Active Directory is enabled or disabled in **Settings** ▶ **Advanced settings**. The functions with regard to compliance can also be enabled or disabled according to FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11.

-

  The wizard for software licensing is opened in **Settings** ▶ **Software licenses**. The licensing wizard will guide the user through the licensing process of the OMNIS Software and offers support for increasing the number of usable instruments.

-

  The size of the local database is displayed under **Settings** ▶ **Database settings**.
  If a local database is used, a backup file of the currently used database can be created manually and the automatic database backup can be enabled or disabled. In addition, the remaining storage capacity of the selected database is displayed. If the database size is critical, information on the occupied space of the local database is also displayed in the title bar of the OMNIS Software.
  Furthermore, the corresponding button can be used to change the operation mode for carrying out service activities. Additional information on the operation mode: *(see "Operation mode – Definition", chapter 6.1.7, page 1233)*
  The connection settings are displayed when an external database is used on a dedicated Microsoft SQL Server in OMNIS Stand-Alone. These details can also be found in the **OMNIS Database Administration** program on the **Overview** tab.

-

  The automatic archiving of samples which is executed at a certain interval is defined in **Settings** ▶ **Scheduler**.

If an external database is used on a dedicated Microsoft SQL Server in OMNIS Stand-Alone, then the **Backup database** and **Automatic database backup** areas are not available. The backup of the database is carried out by an internal IT administrator.
Information on databases in the **OMNIS Client/Server system**: *(see "Database – Definition", chapter 4.6, page 117)*

See also

Advanced settings – Subsection (chapter 5.15.4, page 1205)

Backing up the database (chapter 6.1.3, page 1218)

Database settings – Subsection (chapter 5.15.5, page 1206)

Database – Definition (chapter 4.6, page 117)

Enabling user management (Active Directory) (chapter 4.5.2, page 45)

Enabling user management (OMNIS) (chapter 4.5.3, page 63)

General settings – Subsection (chapter 5.15.3, page 1203)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Database Administration – Actions (chapter 6.1, page 1207)

Setting up a database (OMNIS Stand-Alone) (chapter 4.6.1, page 119)

Setting up notifications (chapter 5.15.1, page 1199)

User management settings – Subsection (chapter 4.5.4, page 66)

User rights – Directory (chapter 4.5.7.4, page 89)

5.15.1 Setting up notifications

Information on the settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

A connection to an e-mail server can be set up in **Settings** ▶ **General settings** ▶ **Notifications**. After a connection has been established successfully, notifications can be sent automatically via e-mail from the OMNIS Software with the **NOTIFY** command.

All the necessary access data can be obtained from the internal IT administrator.

1 Entering the SMTP outgoing mail server

- Enter the host name of the SMTP server that is used for sending e-mails in the **SMTP server** field.

The host name of the SMTP server may only contain ASCII characters **a** to **z** and **A** to **Z**, the numbers **0** to **9** and the hyphen-minus.

2 Entering the TCP Port

- Enter the port of the SMTP server that is used for data transmission in the **TCP port** field.

3 Selecting the encryption type

- Select between **None** or **SSL/TLS** in the selection list.

If **None** is selected, the data is sent to the SMTP server without encryption. If **SSL/TLS** is selected, the data transfer is done with encryption.

4 Entering the user name and the password

- Enter the user name and the password for the SMTP server in the fields **User name** or **Password**.

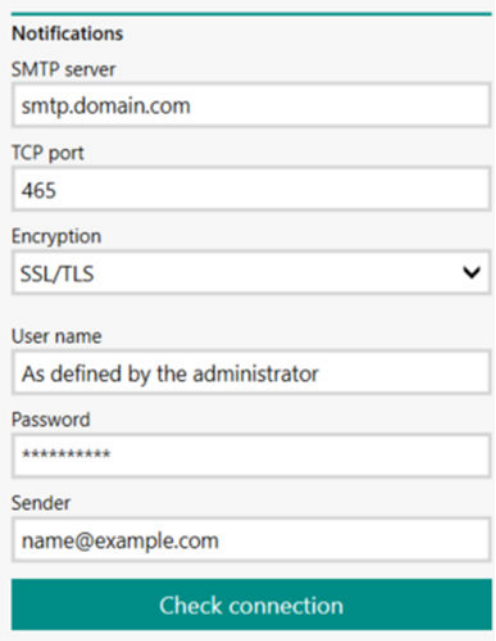
Entering the user name and the password is only necessary, if the SMTP server requires authentication. Otherwise these fields can be left empty.

The password must contain between 6 and 64 characters.

5 Entering a sender

- Enter the e-mail address of the sender with which the notification will be sent in the **Sender** field.

After all these details have been entered, the connection settings are as shown in this sample configuration:



6 Running the connection test

- Validate the values entered against the SMTP server by clicking on **[Check connection]**.

The OMNIS Software sends a test e-mail to the SMTP server. If all the settings are correct, the SMTP server forwards this test e-mail to the e-mail address of the sender entered.

If the sender does not receive a test e-mail, the connection could not be established successfully. If this is the case, check all the notification settings and test the connection again.

If the **Audit Trail** function in the **FDA 21 CFR Part 11 and Eudra-Lex, Volume 4, Annex 11** option is activated, then all of the changes made in the OMNIS Software will be recorded and listed in the Audit Trail. For more information regarding the recording of entries in the Audit Trail, see: *(see "Audit Trail – Directory", chapter 5.14.5, page 1177)*

See also

Advanced settings – Subsection (chapter 5.15.4, page 1205)

Audit Trail – Actions (chapter 5.14, page 1171)

Database settings – Subsection (chapter 5.15.5, page 1206)

General settings – Subsection (chapter 5.15.3, page 1203)

Locking compliance (chapter 4.3, page 39)

NOTIFY – Parameters (chapter 5.11.8.72, page 787)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

User management settings – Subsection (chapter 4.5.4, page 66)

User rights – Directory (chapter 4.5.7.4, page 89)

5.15.2 Scheduler – Subsection

The following functions are available in **Settings** ▶ **Scheduler**:

-

  Create task creates a new task for which an execution time, an execution interval and other parameters can be defined.
-

  Use **Delete task** to delete the selected task.
-

  The properties of the task are displayed in the **Properties** window.

Overview list

The following information is displayed in the overview list:

Name	Name of the task. The name can be modified after opening the task.
Type	Type of task. The following task types can be defined: ▪ Archiving samples
Last run	Time when the task was last executed successfully. **Note:** If the execution of a task was interrupted by an error, then this execution time is not applied. The column still shows the time of the last successful execution.

Next run	Time when the task is scheduled to be executed the next time. The time can be modified after opening the task. **Note:** If a task could not be executed as scheduled (e.g. because the computer is switched off at the time of the next execution), then it will be executed at the next possible time. The following executions are calculated using the defined interval.

See also

Archiving samples (chapter 5.10.4.3, page 255)

Settings – Actions (chapter 5.15, page 1197)

5.15.2.1 Planning task

Planning new task

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*

1 Creating task

- Under **Settings** ▶ **Scheduler**, click on +.

A tab with the new task opens.

2 Defining task

- Define the name of the task in the **Name** field.
- Under **Time period since the most recent modification**, specify which samples are to be taken into account. Only samples with a change date that is older than the time period entered are archived.

The execution of multiple tasks at the same time and for the same samples is not supported. Metrohm recommends defining each task in such a way that it takes other samples into account.

If a task is deleted during its execution, the task is continued until it fails or is terminated. After deleting a task, wait until the scheduled execution time has elapsed before creating a new task for the same samples.

3 Defining an execution time and interval

- Under **Date/Time**, enter the desired time for the first task execution.
- Under **Interval**, enter the interval for the task run.
  Notice: The interval can not be changed later.
- Under **Target folder**, enter the target folder in which the files for the samples and subsamples are to be saved. The target folder must not be read-only. If the defined folder does not already exist, then it will be created during archiving.
- Save the task by clicking on .

The task is saved and executed at the defined time. All samples that fulfill the **Time period since the most recent modification** parameter are exported to the target folder and removed from the database.

If the task could not be executed at the defined time (e.g. because the computer was switched off), then it will be executed as soon as possible. The following executions are calculated using the defined interval.

See also

Archiving Audit Trail (chapter 5.14.9, page 1192)

Audit Trail – Actions (chapter 5.14, page 1171)

Exporting operating procedures and methods (chapter 5.11.1.5, page 393)

Exporting subsample data (chapter 5.10.1.3, page 220)

User rights – Directory (chapter 4.5.7.4, page 89)

5.15.3 General settings – Subsection

Information on the central management of the settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Changed settings for the **User interface**, **Emergency stop function** and **Notifications** will take effect only after a restart of the OMNIS Software.

The following settings are available in **Settings** ▶ **General settings**:

User interface

- The language for the display on the user interface of the OMNIS Software can be selected under **Dialog language**.

Emergency stop function

- If the **Show emergency stop function** check box is enabled, then the button is displayed.
  With the emergency stop, all functional units can be stopped and current determinations can be canceled. Afterwards, the functional units can be moved to a safe status with the OMNIS Software and reinitialized.
  The button is always displayed on top in the user interface. It can be moved around the screen as required.

Include preliminary run test

- If the **Include preliminary run test** check box is enabled, then the preliminary run test is automatically included in all determinations. The preliminary run test will check all selected subsamples together before starting a determination.

Print settings

- An available physical network printer or local printer can be selected under **Default printer**. The selected printer is set as the default printer for printing reports.
  The printer selection is updated each time the **General settings** subsection is opened. If the required printer is not in the selection list, then the correct printer driver must be installed. Only printers that are installed on the computer with the printer drivers of the manufacturer can be used.

Other printers can be selected as **Printer** for manual report creation. Additional information on the options and printer selection when creating reports: *(see "Creating report", chapter 5.10.1.4, page 224)*

- If the **Enable print settings adjustment** check box is enabled, then the following settings can be additionally adjusted during manual report creation: **Copies**, **Double-sided printing** and **Color**. If the **Enable print settings adjustment** check box is disabled, then the defined values for these settings are applied for each print.

Notifications

- A connection to an e-mail server can be set up in this section. After a connection has been successfully established, notifications can be sent automatically via e-mail from the OMNIS Software with the **NOTIFY** command. Additional information on setting up notifications: *(see "Setting up notifications", chapter 5.15.1, page 1199)*

See also

Managing the password (chapter 4.5.8, page 102)

5.15.4 Advanced settings – Subsection

Information on the central management of the settings in the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

The following settings are available in **Settings** ▶ **Advanced settings**:

System

- The language for the output of reports and Audit Trail entries can be selected under **System language**.
- The interval at which the log files are uploaded from the OMNIS Clients to the OMNIS Server can be defined under **Log files upload interval**. The default interval for uploading is 300 seconds.
  For larger OMNIS Client/Server systems, Metrohm recommends increasing the default value of 300 seconds.
- The interval at which the data is synchronized between the OMNIS Client and the OMNIS Server can be defined under **Interval for the synchronization of data**. The default interval for synchronization is 30 seconds.
  For larger OMNIS Client/Server systems, Metrohm recommends increasing the default value of 30 seconds.

User management

- The **User management (OMNIS)** or the **User Management (Active Directory)** can be enabled in this section. Additional information on the activation of user management: *(see "Enabling user management (Active Directory)", chapter 4.5.2, page 45), (see "Enabling user management (OMNIS)", chapter 4.5.3, page 63)(see "Enabling user management (OMNIS)", chapter 4.5.3, page 63)*

Compliance

- The functions for achieving conformity with FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11 can be enabled in this section. Additional information on conformity functions and locking conformity: *(see "Locking compliance", chapter 4.3, page 39)*

See also

Collecting OMNIS system information (chapter 7.3, page 1238)

Managing the password (chapter 4.5.8, page 102)

5.15.5 Database settings – Subsection

The following settings are available in **Settings** ▶ **Database settings**:

Database size

- The size of the current database and the remaining space capacity are displayed in this section when a local database is used.
  If the critical database size is reached, then information is displayed in the title bar of the OMNIS Software.

Backup database

- The database can be backed up manually in this section. Additional information on database backup: *(see "Backing up the database", chapter 6.1.3, page 1218)*

Automatic database backup

- The automatic database backup can be enabled and the settings for it can be defined in this section. Additional information on database backup: *(see "Backing up the database", chapter 6.1.3, page 1218)*

Change operation mode

- The operation mode can be changed in this section. Additional information on the operation modes: *(see "Changing the operation mode", chapter 6.1.8, page 1233)*

See also

Managing the password (chapter 4.5.8, page 102)

6 Maintenance

6.1 OMNIS Database Administration – Actions

You will need local administrator rights in Windows to execute the **OMNIS Database Administration** program.

The following actions can be executed in the tabs, depending on the selected database (local or external database):

- The size of the currently used database, the remaining storage capacity if a local database is used as well as the connection settings if an external database is used are displayed under **Overview**.
  These details can also be found in the OMNIS Software under **Settings** ▶ **Database settings**.

  It is not possible to switch from a local database to an external database in the **OMNIS Client/Server system**. The OMNIS Server must be connected to an external database during the initial installation.
  Instructions for connecting the external database after the initial installation: *(see "Setting up a database (OMNIS Client/Server system)", chapter 4.6.2, page 128)*

- A backup of the currently used database can be created and backup files can be restored under **Back up / Restore**. In addition, the backup files can be checked at any time.
  The local database can also be backed up in the OMNIS Software under **Settings** ▶ **Database settings**.

  A local database from an **OMNIS Stand-Alone** must not be restored in an **OMNIS Client/Server system** or vice versa. The respective formats of the databases are not compatible.

- The database can be updated to a new database version and reset to the factory setting (empty database) under **Update / Reset**.

In the title bar of the program, the corresponding button can be used to change the operation mode for performing service activities. Additional information on the operation mode: *(see "Operation mode – Definition", chapter 6.1.7, page 1233)*

The **Back up / Restore** tab is not available if an external database is used on a dedicated Microsoft SQL Server. Database backup and restoration of the database are carried out by an internal IT administrator.

See also

Backing up the database (chapter 6.1.3, page 1218)

Changing the operation mode (chapter 6.1.8, page 1233)

Database – Definition (chapter 4.6, page 117)

Resetting the local database (OMNIS Stand-Alone and OMNIS Client) (chapter 6.1.5, page 1227)

Restoring the database (chapter 6.1.4, page 1225)

Setting up a database (OMNIS Stand-Alone) (chapter 4.6.1, page 119)

Settings – Actions (chapter 5.15, page 1197)

Updating the database (OMNIS Stand-Alone) (chapter 6.1.1, page 1208)

User rights – Directory (chapter 4.5.7.4, page 89)

6.1.1 Updating the database (OMNIS Stand-Alone)

There are 3 options in the OMNIS Software for updating the database:

- *Updating the database after installing the OMNIS Software*: The database must be updated after the OMNIS Software is installed.
- *Updating the database after restoring the database*: If the database is out of date, the database version must be updated after restoring the database.
- *Updating the database when starting the OMNIS Software*: If the version of the database is out of date, a message is displayed when the OMNIS Software is started.

Information on the database in the **OMNIS Client/Server system**: *Database - Definition*

Information on the **OMNIS Client/Server system**: *OMNIS Client/Server system - Definition*

To perform service activities, a total of 3 operation modes of the OMNIS system must be configured. The update of the database must be carried out for each operation mode separately.

Updating the database after installing the OMNIS Software

Prerequisite:

- The OMNIS Software is installed or updated.
- The Windows user currently logged on has the local administrator rights.
- The required operation mode was selected.
- The software license for starting the OMNIS Software is available. Additional information on the software licenses can be obtained at *http://www.metrohm.com* or from your regional Metrohm representative.

1 Opening the OMNIS Database Administration program

- Enable the check box in the last dialog of the installation wizard of the OMNIS Software.
- Exit installation by clicking on **[Finish]**.

The **OMNIS Database Administration** program is opened and a dialog appears.

2 Updating the database

- Click on **[Update]** in the open dialog to update the database.

This may take several minutes. The current and the new database now have the same version number.

3 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

Updating the database after restoring the database

Prerequisite:

- The **OMNIS Database Administration** program is open.
- Restoring the database is complete.
- The Windows user currently logged on has the local administrator rights.
- The required operation mode was selected.
- The software license for starting the OMNIS Software is available. Additional information on the software licenses can be obtained at *http://www.metrohm.com* or from your regional Metrohm representative.

1 Opening a tab

- Open the **Update / Reset** tab.

2 Updating the database

- Click on the active **[Update]** button to update the database.

This may take several minutes. The current and the new database now have the same version number.

The database version that is to be restored cannot be higher than the database version that is already in use. If the current database version is higher than the database version of the installed OMNIS Software version after restoring the database, then the database cannot be updated anymore. To continue working with the installed OMNIS Software, the database must be reset or an older database version must be restored.

3 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

Message to update the database when starting the OMNIS Software

Prerequisite:

- The required operation mode was selected.
- The Windows user currently logged on has the local administrator rights.
- The software license for starting the OMNIS Software is available. Additional information on the software licenses can be obtained at *http://www.metrohm.com* or from your regional Metrohm representative.

1 Confirming the message

- Confirm the **Database update required** dialog by clicking on **[Update]**.

Another dialog appears with the recommendation to back up the database before carrying out the update.

If the database has already been backed up, continue with step 4 *Updating the database*.

2 Updating the database with a previous backup of the database

- Open the **OMNIS Database Administration** program by clicking on **[Cancel]**.

The **Update / Reset** tab is opened automatically.

No administrator rights are necessary for this step.

3 Backing up the database

- Change to the **Back up / Restore** tab to back up the database.

Additional information about backing up the database: *(see "Backing up the database", chapter 6.1.3, page 1218)*. If an external database (Microsoft SQL Server) is used, the backup of the database is carried out by an internal IT administrator.

4 Updating the database

- Update the database to the latest database version on the **Update / Reset** tab by clicking on **[Update]**.

This may take several minutes. The current and the new database now have the same version number.

5 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

See also

Backing up the database (chapter 6.1.3, page 1218)

Changing the operation mode (chapter 6.1.8, page 1233)

Database – Definition (chapter 4.6, page 117)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operation mode – Definition (chapter 6.1.7, page 1233)

Resetting the local database (OMNIS Stand-Alone and OMNIS Client) (chapter 6.1.5, page 1227)

Restoring the database (chapter 6.1.4, page 1225)

Setting up a database (OMNIS Stand-Alone) (chapter 4.6.1, page 119)

User rights – Directory (chapter 4.5.7.4, page 89)

6.1.2 Updating the database (OMNIS Client/Server system)

To perform service activities, a total of 3 operation modes of the OMNIS system must be configured. To do this, the following instructions must be repeated 3 times for each operation mode.

Additional information on the operation modes: *Definition operation mode*

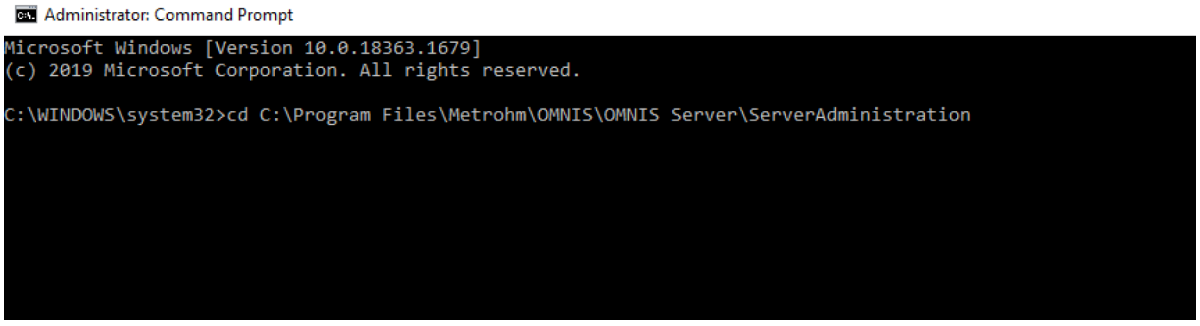
Updating the database on the OMNIS Server

Prerequisite:

- The **OMNIS Client/Server system** is set up.
- The Windows user currently logged on has the local administrator rights.
- A backup of the database has been created.
- The software license for starting the OMNIS Software is available. Further information on the software licenses can be obtained at *www.metrohm.com* or from your regional Metrohm representative.

1 Switching to the OMNIS Server in a command prompt

- Open the Windows start menu.
- Search for the Windows command prompt. Open the context menu by right-clicking and select **Run as administrator**.
- Enter the text **cd** (change directory) followed by a space and then enter the installation pathway of the OMNIS Server (**C:\Program Files\Metrohm\OMNIS\OMNIS Server\ServerAdministration** by default).
- Confirm the entry with **[Enter]**.



2 Configuring the connection via command prompt (optional)

All the necessary access data can be obtained from the internal IT administrator.

Encryption is activated by default for the connection between the OMNIS server and the database server. The certificate to be used must have been issued by a trusted certificate authority. If required (e.g. for use in a test environment), you can also work with self-signed certificates by adding the parameter **";TrustServerCertificate=true"** for the definition of the database connection parameters. For safety reasons, Metrohm recommends not using self-signed certificates in production environments, as they do not offer high safety standards.

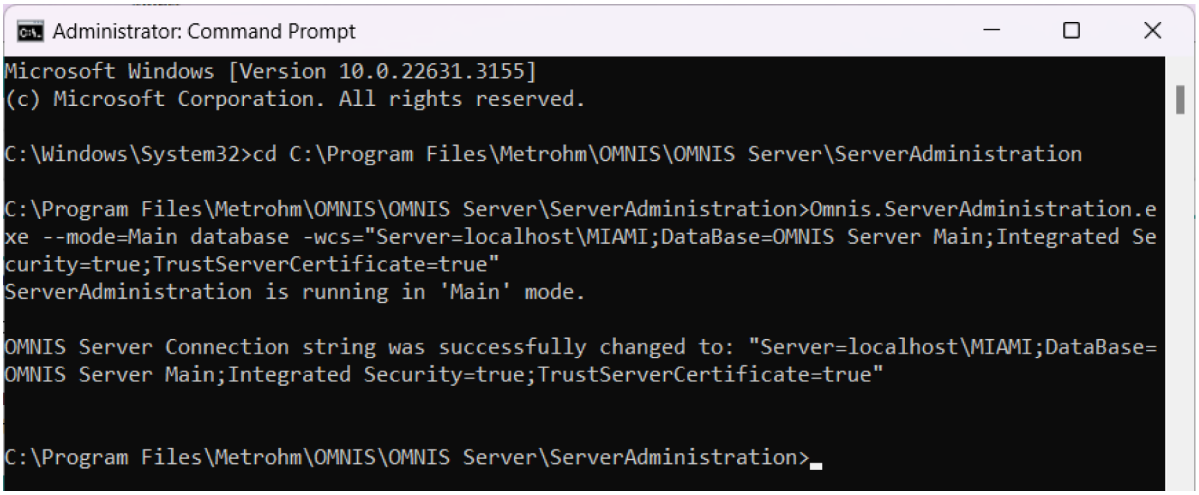
If the Windows authentication mode was selected in the following instructions *Preparing the database (OMNIS Client/Server system)* **(recommended)**:

- Prepare the following information:
  - Name of the computer in the network on which the Microsoft SQL Server is running (e.g. 001-CMP-00000).
  - Instance of the Microsoft SQL Server (e.g. METROHM-SERVER).
  - Name of the database (Main, OQ-FS or C1-PV) on the Microsoft SQL Server (e.g. OMNISServer).
  - Specification of the user authentication. If Integrated Security is set to true, then Windows authentication is used.
  - Specification of the certificate type (self-signed or acquired from a trusted certificate authority).
- Enter the following text line in the command prompt, replacing the individual text parts with your own specific information:
  Omnis.ServerAdministration.exe --mode=**Name of the operation mode** database -wcs="Server=**Name of the computer****Server instance**;DataBase=**Name of the database**;IntegratedSecurity=**true**"
  Example for the entry in the Main operation mode:
  - Omnis.ServerAdministration.exe --mode=Main database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerMain;IntegratedSecurity=true"

  Example for the entry in the OQ-FS operation mode in the second run of the instructions:
  - Omnis.ServerAdministration.exe --mode=OQ-FS database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerOQ-FS;IntegratedSecurity=true"

  Example for the entry in the C1-PV operation mode in the third run of the instructions:
  - Omnis.ServerAdministration.exe --mode=C1-PV database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerC1-PV;IntegratedSecurity=true"

- Confirm the entry with **[Enter]**.



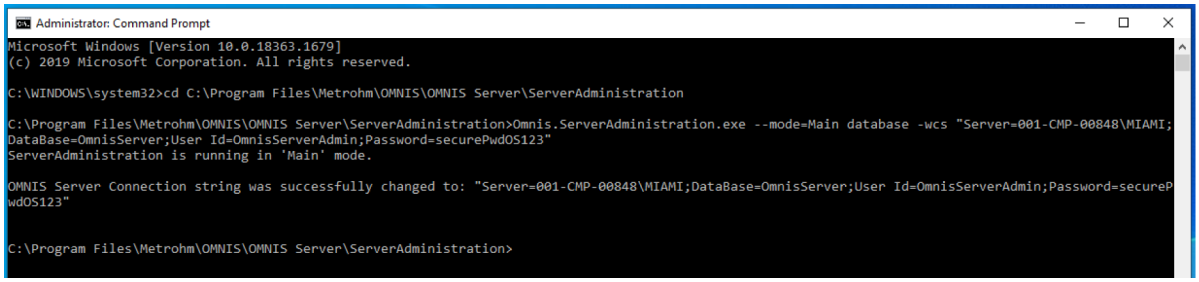
If the SQL server authentication mode was selected in the following instructions *Preparing the database (OMNIS Client/Server system)*:

- Prepare the following information:
  - Name of the computer in the network on which the Microsoft SQL Server is running (e.g. 001-CMP-00000).
  - Instance of the Microsoft SQL Server (e.g. METROHM-SERVER).
  - Name of the database (Main, OQ-FS or C1-PV) on the Microsoft SQL Server (e.g. OMNISServer).
  - Name of the user for the access to the database (e.g. OMNISServerAdmin).
  - Password of the user for access to the database (e.g. OMNISServerAdminPassword).
  - Specification of the certificate type (self-signed or acquired from a trusted certificate authority).

- Enter the following text line in the command prompt, replacing the individual text parts with your own specific information:
  Omnis.ServerAdministration.exe --mode=**Name of the operation mode** database -wcs="Server=**Name of the computer\Server instance**;DataBase=**Name of the database**;User Id=**Name of the user**;Password=**Password of the user**"
  Example for the entry in the Main operation mode:
  – Omnis.ServerAdministration.exe --mode=Main database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerMain;User ID=OMNISServerAdmin;Password=OMNISServerAdminPassword"

  Example for the entry in the OQ-FS operation mode in the second run of the instructions:
  – Omnis.ServerAdministration.exe --mode=OQ-FS database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerOQ-FS;User ID=OMNISServerAdmin;Password=OMNISServerAdminPassword"

  Example for the entry in the C1-PV operation mode in the third run of the instructions:
  – Omnis.ServerAdministration.exe --mode=C1-PV database -wcs="Server=001-CMP-00000\METROHM-SERVER;DataBase=OMNISServerC1-PV;User ID=OMNISServerAdmin;Password=OMNISServerAdminPassword"
- Confirm the entry with **[Enter]**.

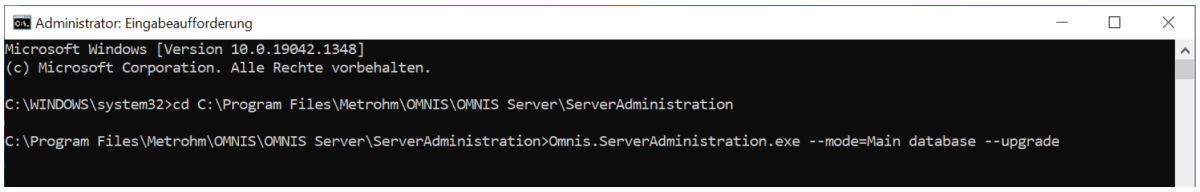


The command prompt confirms that the connection was successfully changed.

3 Starting the update via the command prompt

- Prepare the following information:
  – Name of the database (Main, OQ-FS or C1-PV) on the Microsoft SQL Server (e.g. OMNIS Server).

- Enter the following text line in the command prompt, replacing the text part **ModeName** with the specific name of the operation mode:
  Omnis.ServerAdministration.exe --mode=ModeName database --upgrade
  Example for the entry in the Main operation mode:
  Omnis.ServerAdministration.exe --mode=Main database --upgrade
  Example for the entry in the OQ-FS operation mode in the second run of the instructions: Omnis.ServerAdministration.exe --mode=OQ-FS database --upgrade
  Example for the entry in the C1-PV operation mode in the third run of the instructions: Omnis.ServerAdministration.exe --mode=C1-PV database --upgrade
- Confirm the entry with **[Enter]**.

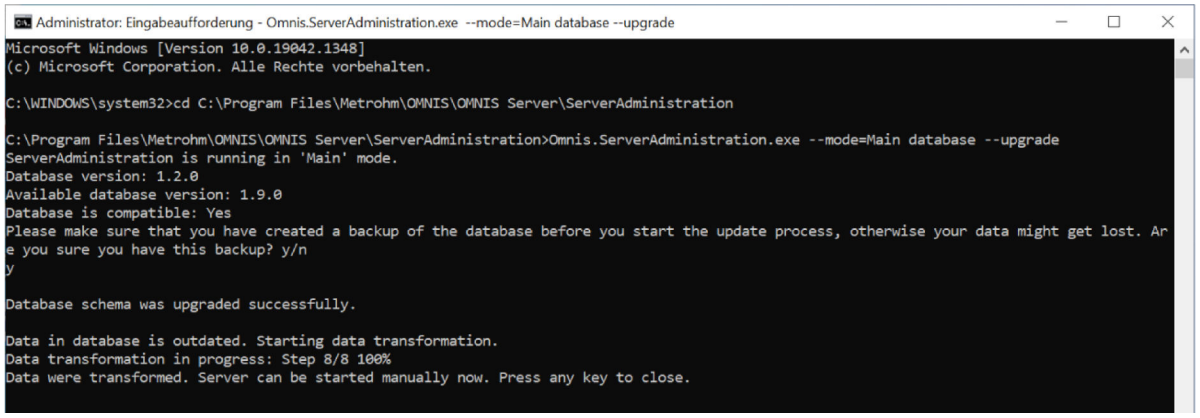


The command prompt confirms the currently installed version and the version that is needed to support the new OMNIS Server version.

4 Updating the database

Ensure that a backup of the database is saved to avoid a potential loss of data.

- Confirm in the command prompt that a backup of the database has been created. To do so, enter the letter **y** and confirm with **[Enter]**.



The command prompt confirms that the database schema and the data were successfully updated.

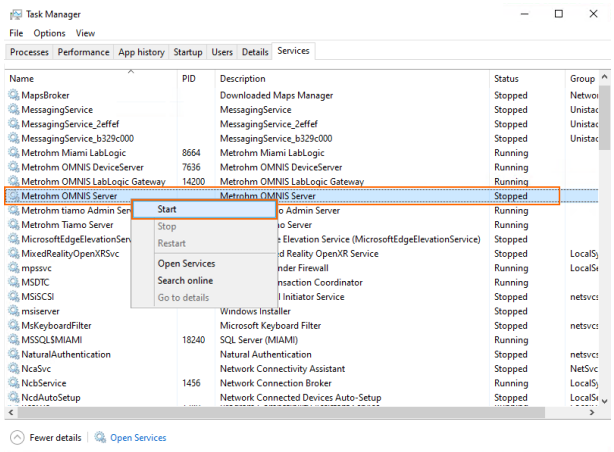
If the database was not updated successfully, load the backup of the database again and repeat the process. Further information on the error can be found in the log file. Contact your regional Metrohm representative if the error recurs multiple times.

5 Starting the service for the OMNIS Server

- Right-click on the Windows task bar and select **[Task Manager]** in the selection list.
- Right-click on the applicable service on the **Services** tab:
  Main operation mode:
  – Service **Metrohm OMNIS Server**

  OQ-FS operation mode in the second run of the instructions:
  – Service **Metrohm OMNIS Server_OQ-FS**

  C1-PV operation mode in the third run of the instructions:
  – Service **Metrohm OMNIS Server_C1-PV**
- Select **[Start]** in the selection list.



The service is started.

The following reasons may apply if the **Metrohm OMNIS Server** (**Metrohm OMNIS Server_OQ-FS** or **Metrohm OMNIS Server_C1-PV)** service cannot be started:

- The database schema is not up-to-date or not compatible with the OMNIS Server.
- The connection to the database could not be established.

If this is the case, check the data entered in the command prompt according to step 2 (Starting the update via the command prompt). Enter the data for the connection again, if applicable. Contact your internal IT administrator if this error continues to occur.

6 Repeating the instructions

- Repeat all the steps in the second and third run for the corresponding operation mode.

7 Updating OMNIS Clients

Update the OMNIS Software for the connected OMNIS Clients within 48 hours: *Updating the OMNIS Software*

See also

Database – Definition (chapter 4.6, page 117)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Database Administration – Actions (chapter 6.1, page 1207)

Resetting the local database (OMNIS Stand-Alone and OMNIS Client) (chapter 6.1.5, page 1227)

Restoring the database (chapter 6.1.4, page 1225)

User rights – Directory (chapter 4.5.7.4, page 89)

6.1.3 Backing up the database

If a local database (Microsoft SQL Server Express) is used, the user can carry out the manual backup of the database in the OMNIS Software or in the OMNIS Database Administration. The automatic database backup is carried out exclusively in the OMNIS Software.

- *Back up the database from the OMNIS Software*
- *Back up database from the OMNIS Database Administration*
- *Automatic database backup from the OMNIS Software*

If an external database is used, the database backup from the OMNIS Software and the **Back up / Restore** tab in the **OMNIS Database Administration** program are not available in OMNIS Stand-Alone. The backup of the database must be carried out by an internal IT administrator.

Information on the database in the **OMNIS Client/Server system**: *Database - Definition*
Information on the **OMNIS Client/Server system**: *OMNIS Client/Server system - Definition*

To perform service activities, a total of 3 operation modes of the OMNIS system must be configured. The backup of the database must be carried out for each operation mode separately.

Backing up the database in the OMNIS Software

Prerequisite:

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The user has the necessary rights. Additional information on user rights: *User rights – Directory*
- The local database (Microsoft SQL Server Express) is installed.
- The OMNIS Software is open.
- The required operation mode was selected.

1 Selecting the work area

- In the **Settings** work area, open the **Database settings** subsection.

2 Defining the Target folder

- Select a target folder by clicking in the **Target folder** field. Alternatively, enter the target folder path in which the backup file is saved.

  Write permission is required to save data to the target folder. When saving on a network drive, either the name of the network drive (e.g. Z:\) or the UNC path (e.g. \\server name\share name\path) can be entered.

3 Entering the file name

- Enter the name under which the backup file is to be saved in the **File name** field.

The following special characters and character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

All time indications are converted into the Coordinated Universal Time (UTC±00:00) when saving. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.

4 Backing up the database

- Back up the database by clicking on **[Back up]**.

The backup file is checked and stored in the defined target folder. This may take several minutes.

By default, the backup file is stored in the default directory: **...\Metrohm\OMNIS\MSSQL*XX*.MIAMI\MSSQL\Backup**

The value ***XX*** and the exact directory path can vary, depending on the installed version of the Microsoft SQL Server.

When the OMNIS Software is closed and opened, the default directory is shown again.

Once the backup file has been saved, a message appears.

If the database file is invalid or damaged, the file name is extended by the ending **_corrupted** and an error message appears.

Saving the backup file

Backup files of the database can be saved on a network drive or on the same drive, on which the database is installed. If files are saved locally, data may be lost if the computer crashes or the hard drive becomes defective. Metrohm recommends saving or copying backup files to an external storage medium at regular intervals.

5 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

Backing up the database from the OMNIS Database Administration

Prerequisite:

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The local database (Microsoft SQL Server Express) is installed.
- The required operation mode was selected.
- The Windows user currently logged on has the local administrator rights.

1 Executing the OMNIS Database Administration program

- Start the **OMNIS Database Administration** program via the program directory (**...\Metrohm\OMNIS\Desktop** by default).
  or
- Run the **OMNIS Database Administration** program from the Windows start menu.

2 Opening a tab

- Open the **Back up / Restore** tab.

3 Defining the Target folder

- Select a target folder by clicking in the **Target folder** field. Alternatively, enter the target folder path in which the backup file is saved.

Write permission is required to save data to the target folder.
When saving on a network drive, either the name of the network drive (e.g. Z:\) or the UNC path (e.g. \\server name\share name\path) can be entered.

4 Entering the file name

- Enter the name under which the backup file is to be saved in the **File name** field.

The following special characters and character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9
All time indications are converted into the Coordinated Universal Time (UTC±00:00) when backing up. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.

5 Backing up the database

- Back up the database by clicking on **[Back up]**.

The backup file is checked and stored in the defined target folder. This may take several minutes.

By default, the backup file is stored in the default directory: **...\Metrohm\OMNIS\MSSQL*XX*.MIAMI\MSSQL\Backup**
The value ***XX*** and the exact directory path can vary, depending on the installed version of the Microsoft SQL Server.

Once the backup file has been saved, a message appears.

If the database file is invalid or damaged, the file name is extended by the ending **_corrupted** and an error message appears.

Saving the backup file
Backup files of the database can be saved on a network drive or on the same drive, on which the database is installed. If files are saved locally, data may be lost if the computer crashes or the hard drive becomes defective. Metrohm recommends saving or copying backup files to an external storage medium at regular intervals.

6 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

Automatic database backup from the OMNIS Software

Prerequisite:

- The necessary software licenses and function licenses are enabled. Additional information: *Metrohm Knowledge Base*
- The user has the necessary rights. Additional information on user rights: *User rights – Directory*
- The local database (Microsoft SQL Server Express) is installed.
- The required operation mode was selected.

1 Selecting the work area

- In the **Settings** work area, open the **Database settings** subsection.

2 Enabling automatic database backup

- Activate the **Automatic database backup** function by clicking on the check box.

The settings for the automatic database backup can be defined.

3 Defining the date and time

- Click on 15 to define the date for the automatic database backup.
- Select the hours and minutes in the selection list.

4 Defining the Interval

- Enter the number of the interval until the next database backup.
- Select Week(s), Day(s) or Hour(s) in the selection list.

5 Defining the Target folder

- Select a target folder by clicking in the **Target folder** field. Alternatively, enter the target folder path in which the backup file is saved.

By default, the default directory is selected as the target folder: **...\Metrohm\OMNIS\MSSQL*XX*.MIAMI\MSSQL\Backup**

The value ***XX*** and the exact directory path can vary, depending on the installed version of the Microsoft SQL Server.

If a network drive is selected for the target folder, then the two entry fields **User name** and **Password** will appear. When saving on a network drive, either the name of the network drive (e.g. Z:\) or the UNC path (e.g. \\server name\share name\path) can be entered.

6 Entering the file name

- Enter the name under which the backup file is to be saved in the **File name** field.

The following special characters and character strings may not be used: >, <, :, ", /, \, |, *, ? and CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

All time indications are converted into the Coordinated Universal Time (UTC±00:00) when saving. This is indicated by a Z (no deviation from UTC) at the end of the time indication (e.g. 2018-04-25 11:43:08Z). This time format may differ from the local time on the computer.

7 Entering the User name (optional)

- Enter the Windows user name in the **User name** field.

The Windows user requires write permission for the target folder.

8 Entering the Password (optional)

- Enter the password for the Windows user in the **Password** field.

9 Saving the settings

- Save the defined settings by clicking on **[Apply]**.

The backup file is checked automatically at the requested time and saved in the defined target folder.

If the database file is invalid or damaged, the file name is extended by the ending **_corrupted** and an error message appears.

Saving the backup

If the computer is switched off at the time of the automatic database backup, then the automatic database backup will be carried out as soon as the OMNIS Software is opened once again.

10 Changing the operation mode

- Change the operation mode by following these instructions: *Changing the operation mode*
- Then repeat all the steps for each operation mode.

See also

Audit Trail – Directory (chapter 5.14.5, page 1177)

Changing the operation mode (chapter 6.1.8, page 1233)

Database – Definition (chapter 4.6, page 117)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

Operation mode – Definition (chapter 6.1.7, page 1233)

Resetting the local database (OMNIS Stand-Alone and OMNIS Client) (chapter 6.1.5, page 1227)

Restoring the database (chapter 6.1.4, page 1225)

Updating the database (OMNIS Stand-Alone) (chapter 6.1.1, page 1208)

User rights – Directory (chapter 4.5.7.4, page 89)

6.1.4 Restoring the database

If an external database is used, the **Back up / Restore** tab in the **OMNIS Database Administration** program is not available. The database must be restored by an internal IT administrator.

A local database from an **OMNIS Stand-Alone** must not be restored in an **OMNIS Client/Server system** or vice versa. The respective database formats are not compatible.

Information on the database in the **OMNIS Client/Server system**: *(see "Database – Definition", chapter 4.6, page 117)*

Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

To perform service activities, a total of 3 operation modes of the OMNIS system must be configured. The restoration of the database must be carried out for each operation mode separately.

Prerequisite:

- The local database (Microsoft SQL Server Express) is installed.
- The required operation mode was selected.
- The database to be restored does not originate from an OMNIS software version that is newer than the currently installed OMNIS software version.
- The OMNIS Software is closed.
- The user has the necessary rights. Additional information on user rights: *(see "User rights – Directory", chapter 4.5.7.4, page 89)*
- The Windows user currently logged on has the local administrator rights.

1 Executing the OMNIS Database Administration program

- Start the **OMNIS Database Administration** program via the program directory (**...\Metrohm\OMNIS\Desktop** by default).
  or
- Run the **OMNIS Database Administration** program from the Windows start menu.

2 Opening a tab

- Open the **Back up / Restore** tab.

3 Selecting the database file

- Click on **[Select database file]** to open the default directory: **...\Metrohm\OMNIS\MSSQL*XX*.MIAMI\MSSQL\Backup**.
  The value ***XX*** and the exact directory path can vary, depending on the installed version of the Microsoft SQL Server.
- Select the desired backup file.
- Click **[Open]** to confirm the selection.

The selected database file is displayed in the **OMNIS Database Administration**.

4 Verifying the database file (optional)

- Click on **[Verify database file]** to verify the database file.

A message appears once the database file has been verified.

An error message appears if the database file is invalid or damaged. The file cannot be used to restore the database.

A database file can be verified at any time, regardless of whether the database is to be restored.

5 Restoring the database

- Restore the database from the backup file by clicking on **[Restore]**.
- Confirm the following dialog by clicking on **[Continue]**.

The database is restored from the backup file. Depending on the size of the database, this process can take several minutes to several hours.

A message appears once the database has been restored.

6 Changing the operation mode

- Change the operation mode by following these instructions: *(see "Changing the operation mode", chapter 6.1.8, page 1233)*
- Then repeat all the steps for each operation mode.

The database version might have to be updated after restoring the database. Additional information on updating the database: *(see "Updating the database (OMNIS Stand-Alone)", chapter 6.1.1, page 1208)*

See also

Backing up the database (chapter 6.1.3, page 1218)

Changing the operation mode (chapter 6.1.8, page 1233)

Database – Definition (chapter 4.6, page 117)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Database Administration – Actions (chapter 6.1, page 1207)

Operation mode – Definition (chapter 6.1.7, page 1233)

Resetting the local database (OMNIS Stand-Alone and OMNIS Client) (chapter 6.1.5, page 1227)

Setting up a database (OMNIS Stand-Alone) (chapter 4.6.1, page 119)

Updating the database (OMNIS Stand-Alone) (chapter 6.1.1, page 1208)

User rights – Directory (chapter 4.5.7.4, page 89)

6.1.5 Resetting the local database (OMNIS Stand-Alone and OMNIS Client)

If you reset the database, then all of the data in the local database (samples, subsamples, operating procedures, methods, etc.), the device assignments, and the connected instruments with their settings are lost.
Metrohm recommends backing up the existing local database before resetting. Database backup must be carried out by an internal IT administrator if an external database is used.
Additional information on database backup: *(see "Backing up the database", chapter 6.1.3, page 1218)*

Information on the database in the **OMNIS Client/Server system**: *(see "Database – Definition", chapter 4.6, page 117)*
Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

To perform service activities, a total of 3 operation modes of the OMNIS system must be configured. To do this, the following instructions must be repeated 3 times for each operation mode.

Prerequisite:

- The OMNIS Software is closed.
- The Windows user currently logged on has the local administrator rights.

- The required operation mode was selected.

1 Starting the OMNIS Database Administration

- The following options exist for starting the **OMNIS Database Administration** program:
  - Start the **OMNIS Database Administration** program via the program directory (**...\Metrohm\OMNIS\Desktop** by default).
  - Run the **OMNIS Database Administration** program from the Windows start menu.

2 Opening a tab

- Open the **Update / Reset** tab.

3 Resetting the local database

- Click on **[Reset]** to reset the local database to the factory setting.
- Click on **[Continue]** to confirm the message.

The local database will be reset to factory settings (empty database). This may take several minutes.

Once the local database has been reset, a message appears.

4 Changing the operation mode

- Change the operation mode by following these instructions: *(see "Changing the operation mode", chapter 6.1.8, page 1233)*
- Then repeat all the steps for each operation mode.

See also

Backing up the database (chapter 6.1.3, page 1218)

Changing the operation mode (chapter 6.1.8, page 1233)

Database – Definition (chapter 4.6, page 117)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Database Administration – Actions (chapter 6.1, page 1207)

Operation mode – Definition (chapter 6.1.7, page 1233)

Restoring the database (chapter 6.1.4, page 1225)

Setting up a database (OMNIS Stand-Alone) (chapter 4.6.1, page 119)

Updating the database (OMNIS Stand-Alone) (chapter 6.1.1, page 1208)

User rights – Directory (chapter 4.5.7.4, page 89)

6.1.6 Resetting the database (OMNIS Client/Server system)

To perform service activities, a total of 3 operation modes of the OMNIS system must be configured. To do this, the following instructions must be repeated 3 times for each operation mode.

When a reset is carried out, all the data in the database (samples, subsamples, operating procedures, methods, etc.), device assignments, and connected instruments with their settings are lost.
Metrohm recommends backing up the existing database before the reset. Database backup must be carried out by an internal IT administrator if an external database is used.
Additional information on database backup: *(see "Backing up the database", chapter 6.1.3, page 1218)*

Information on the database in the **OMNIS Client/Server system**: *(see "Database – Definition", chapter 4.6, page 117)*
Information on the **OMNIS Client/Server system**: *(see "OMNIS Client/Server system – Definition", chapter 4.1, page 13)*

Prerequisite:

- The **OMNIS Client/Server system** is set up.
- All the OMNIS Clients are closed and no process associated with them is being carried out (e.g. deleting, archiving, removing).
- The Windows user currently logged on has the local administrator rights.

1 Stopping the service for the OMNIS Server

- Right-click on the Windows task bar and select **[Task Manager]** in the selection list.
- Right-click on the applicable service on the **Services** tab:
  For the Main operation mode:
  – Service **Metrohm OMNIS Server**

  For the OQ-FS operation mode:
  – Service **Metrohm OMNIS Server_OQ-FS**

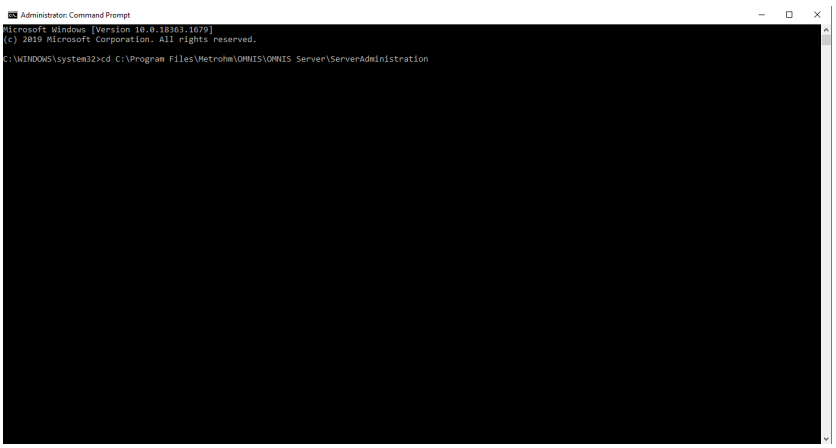
  For the C1-PV operation mode:
  – Service **Metrohm OMNIS Server_C1-PV**
- Select **[Stop]** in the selection list.

The corresponding service is stopped.

2 Switching to the OMNIS Server in a command prompt

- Open the Windows start menu.

- Search for the Windows command prompt. Open the context menu by right-clicking and select **Run as administrator**.
- Enter the text **cd** (change directory) followed by a space and then enter the installation pathway of the OMNIS Server (**C:\Program Files\Metrohm\OMNIS\OMNIS Server\ServerAdministration** by default).
- Confirm the entry with **[Enter]**.

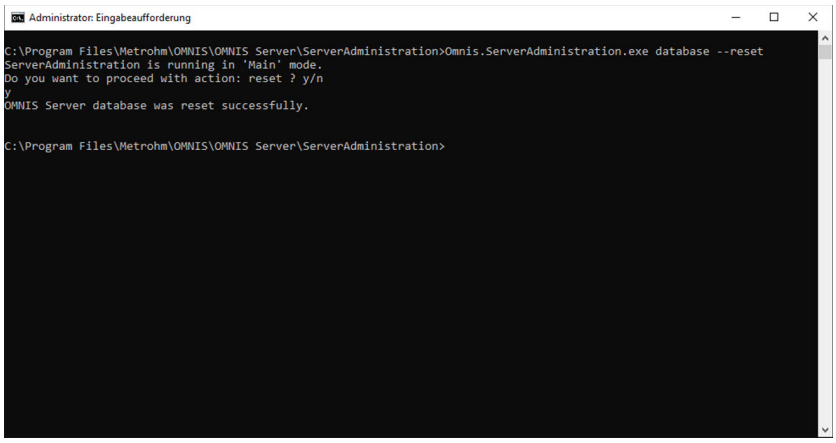


3 Resetting the database

- Enter the following text in the command prompt:
  Example for the entry in the Main operation mode:
  – Omnis.ServerAdministration.exe --mode=Main database --reset

  Example for the entry in the OQ-FS operation mode:
  – Omnis.ServerAdministration.exe --mode=OQ-FS database --reset

  Example for the entry in the C1-PV operation mode:
  – Omnis.ServerAdministration.exe --mode=C1-PV database --reset
- Confirm the entry with **[y]**.



The command prompt confirms that the database was successfully reset.

4 Resetting the databases of all the OMNIS Clients

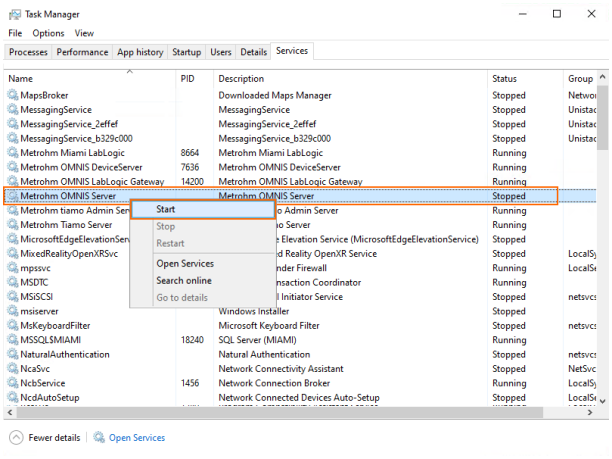
- Reset the local databases of all the OMNIS Clients by following these instructions: *(see "Resetting the local database (OMNIS Stand-Alone and OMNIS Client)", chapter 6.1.5, page 1227)*

5 Starting the service for the OMNIS Server

- Right-click on the Windows task bar and select **[Task Manager]** in the selection list.
- Right-click on the applicable service on the **Services** tab:
  For the Main operation mode:
  - Service **Metrohm OMNIS Server**

  For the OQ-FS operation mode:
  - Service **Metrohm OMNIS Server_OQ-FS**

  For the C1-PV operation mode:
  - Service **Metrohm OMNIS Server_C1-PV**
- Select **[Start]** in the selection list.



The corresponding service is started.

The following reasons may apply if the **Metrohm OMNIS Server** (**Metrohm OMNIS Server_OQ-FS** or **Metrohm OMNIS Server_C1-PV)** service cannot be started:

- The database schema is not up-to-date or not compatible with the OMNIS Server.
- The connection to the database could not be established.

If this is the case, check the data entered in the command prompt according to step 3 (Resetting the database). Enter the data for the connection again, if applicable. Contact your internal IT administrator if this error continues to occur.

6 Enabling user management

- Enable user management by following these instructions: *(see "Enabling user management (Active Directory)", chapter 4.5.2, page 45), (see "Enabling user management (OMNIS)", chapter 4.5.3, page 63)*

If the database was reset in Main operation mode, the software license must also be enabled. Then all the OMNIS Clients must be added to the **OMNIS Client/Server system** again.

See also

Backing up the database (chapter 6.1.3, page 1218)

Changing the operation mode (chapter 6.1.8, page 1233)

Changing the operation mode (chapter 6.1.8, page 1233)

Database – Definition (chapter 4.6, page 117)

OMNIS Client/Server system – Definition (chapter 4.1, page 13)

OMNIS Database Administration – Actions (chapter 6.1, page 1207)

Operation mode – Definition (chapter 6.1.7, page 1233)

Operation mode – Definition (chapter 6.1.7, page 1233)

Restoring the database (chapter 6.1.4, page 1225)

Setting up a database (OMNIS Stand-Alone) (chapter 4.6.1, page 119)

Updating the database (OMNIS Stand-Alone) (chapter 6.1.1, page 1208)

User rights – Directory (chapter 4.5.7.4, page 89)

6.1.7 Operation mode – Definition

An **operation mode** in the OMNIS Software refers to a way in which the OMNIS System is configured. This setting applies to the OMNIS Software, the database as well as the services and ports used. The different operation modes enable the service activities on the OMNIS System (e.g. initial qualification or maintenance). To do this, the operation mode can be changed in the **OMNIS Database Administration** program or in the OMNIS Software under **Settings** ▶ **Database settings**.

The following operation modes are available:

- **Main**: Operation mode for the regular work with the OMNIS Software.
- **C1-PV**: Operation mode for the service check of the functioning of the hardware.
- **OQ-FS**: Operation mode for the service check of the functioning of the software.

In the **OMNIS Client/Server system** the operation mode can be selected for each OMNIS Client separately. The setting does not depend on the connected OMNIS Server. The configuration of the operation modes of the OMNIS Client and the OMNIS Server must always be identical, so that no configuration problems occur.

See also

Changing the operation mode (chapter 6.1.8, page 1233)

6.1.8 Changing the operation mode

To carry our service activities the operation mode of the OMNIS Software can be changed as follows:

Prerequisite:

- The currently logged in Windows user has access to the folder in which the system files for the OMNIS Software are stored: **...ProgramData \Metrohm\OMNIS**

- If the operation mode is changed via the **OMNIS Database Administration** program:
  - The Windows user currently logged on has the local administrator rights.
  - The OMNIS Software is closed and no process is being carried out (e.g. deleting, archiving, removing).
- If the operation mode is changed in the OMNIS Software:
  - The user has the necessary rights. Further information on user rights: *User rights - Directory*

1 Opening the view to change the operation mode

- Start the **OMNIS Database Administration** program. Open the dialog for changing the operation mode by clicking on the button in the title bar on which the current operation mode is being displayed.
  or
- Open the **Settings** ▶ **Database settings** subsection in the OMNIS Software.

2 Changing the operation mode

- Select the required operation mode in the selection list:
  - **Main**: Operation mode for the regular work with the OMNIS Software.
  - **C1-PV**: Operation mode for the service check of the functioning of the hardware.
  - **OQ-FS**: Operation mode for the service check of the functioning of the software.
- Confirm the selection with **[Change]**.

The selected operation mode is displayed in the title bar highlighted with a color.

If the operation mode has been changed in the OMNIS Software, the computer must be restarted for the change to become active.

See also

Operation mode – Definition (chapter 6.1.7, page 1233)

6.2 Sending OMNIS environment information

The OMNIS environment information can be sent directly from the OMNIS Software before a planned service appointment or if requested by Metrohm AG.

Sending OMNIS environment information can only be done in the Main operation mode. Further information on the operation modes: *(see "Changing the operation mode", chapter 6.1.8, page 1233)*

Prerequisite:

- The OMNIS Software is installed.
- An Internet connection is available.
- The Main operation mode was selected.

1 Sending OMNIS environment information

- After clicking on • • • in the title bar of the OMNIS Software, select the **[Send OMNIS environment information]** function in the selection list.

  The **[Send OMNIS environment information]** function can only be selected if an initial license or an additional software license or function license was activated after the installation of the OMNIS Software.

The OMNIS environment information is automatically sent to the Metrohm license server in encrypted form.

In case there is no internet connection, a message appears and the OMNIS environment information is saved as an eiu file on the desktop. This file must be sent to the Metrohm license server from another computer with an internet connection via the following link: *https://activation.metrohm.com/environment-information-update*

Additional information on data storage in the OMNIS Software at: *OMNIS Software – Licensing process*.

See also

Changing the operation mode (chapter 6.1.8, page 1233)

Collecting OMNIS system information (chapter 7.3, page 1238)

OMNIS Software – Faults (chapter 7.1, page 1236)

Operation mode – Definition (chapter 6.1.7, page 1233)

7 Malfunctions and troubleshooting

7.1 OMNIS Software – Faults

In the event of a system fault, a corresponding error message is displayed in the OMNIS Software. If the fault cannot be rectified by applying the measures suggested in the error message, contact must be made with the regional Metrohm representative.

For an overall picture of the system status and the instrument status, it is necessary to collect the information of the system and of the affected instruments and send it to the regional Metrohm representative. The procedure for this differs according to whether or not the OMNIS Software can still be opened.

Faults and the OMNIS Software can still be opened

- The instrument data, the instrument log files and the OMNIS environment information (config.xml) are collected with the **OMNIS system information** function. A ZIP file is then created which has to be sent to the regional Metrohm representative by e-mail (this does not happen automatically).

Faults and the OMNIS Software cannot be opened

- All the available information is collected with the **OMNIS InfoZipper** program. A ZIP file is then created which has to be sent to the regional Metrohm representative by e-mail (this does not happen automatically).

See also

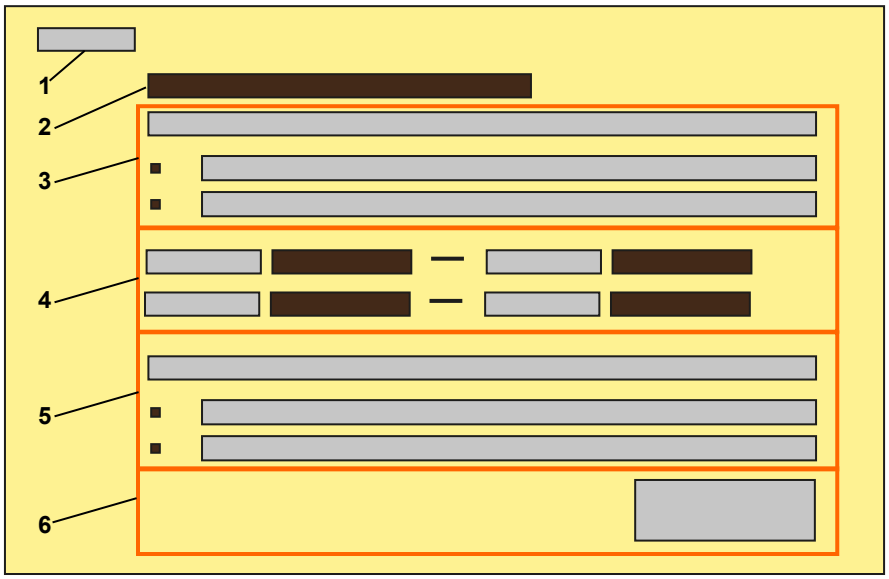
Collecting OMNIS system information (chapter 7.3, page 1238)

Collecting instrument log files (chapter 7.4, page 1241)

Sending OMNIS environment information (chapter 6.2, page 1235)

7.2 Error messages – Concept

Error messages describe the causes and the possibilities for eliminating a fault. Error messages can consist of different information elements that are used in various combinations depending on the error.



1 Error number
The error number is used as an identification feature of a fault and should be specified when contacting the Metrohm representative.

2 Message header
The header provides the user with brief information regarding the type of fault (e.g., **Determination canceled**).

3 Description of causes
This information element describes the type, the effect and the cause of the fault. If the fault has more than one cause, then they are specified in list form.

4 Program variables
The additional auxiliary information that is available during the run time regarding the fault is displayed in this area (e.g., the names of the affected instruments and functional units or the operating procedures and methods that are used). Depending on the fault, a list is compiled. The individual pieces of information are separated from one another by hyphens.

5 Options for troubleshooting
This information element contains supporting instructions for eliminating the fault. If more than one alternative exists or if more than one step is necessary for eliminating the fault, then these will be specified in list form.

6 Buttons
In the case of most error messages, the **[OK]** button is used to close the message. In addition, other buttons may also be present, the function of which is described in the error message itself.

In the event of long fault messages, use the scroll bar on the right-hand message edge to navigate through the message content.

See also

OMNIS Software – Faults (chapter 7.1, page 1236)

7.3 Collecting OMNIS system information

The OMNIS system information is directly collected from the OMNIS Software.

In case of faults where the OMNIS Software cannot be opened, the OMNIS system information must be collected with the **OMNIS InfoZipper** program: *(see "OMNIS InfoZipper", page 1238)*

Collecting OMNIS system information from the OMNIS Software

1 Collecting OMNIS system information

After clicking on • • • in the title bar of the OMNIS Software, select the **[Collect OMNIS system information]** function in the selection list.

When collecting OMNIS system information in the OMNIS Software, all the backup files of the connected instruments are created again and the existing data is overwritten. The existing instrument log files and the OMNIS environment information (config.xml) are only collected.

The collection of the data may take several minutes. Once the OMNIS system information is collected, the desktop opens where the ZIP file was stored.

2 Sending the ZIP file to the regional Metrohm representative

A ZIP file with the OMNIS system information in the following format is stored on the desktop:
'OMNIS_Info_YYYYMMDD_hhmmss_mmm.zip'
YYYY = Year, **MM** = Month; **DD** = Day; **hh** = Hour; **mm** = Minute; **ss** = Second; **mmm** = Millisecond

- Send the ZIP file created on the desktop by e-mail to the regional Metrohm representative.

OMNIS InfoZipper

You will need local administrator rights in Windows to execute the **OMNIS InfoZipper** program. If the **OMNIS InfoZipper** is executed without administrator rights, the collected information is incomplete.

If instruments are affected by a fault, the instrument log files of the affected instruments must first be collected before the log files are collected. Additional information on collecting instrument log files: *(see "Collecting instrument log files", chapter 7.4, page 1241)*

The procedure for collecting the log files differs depending on from where the **OMNIS InfoZipper** program was started.

Running the OMNIS InfoZipper program from an error message

1 Collecting log files

- Click on the **[Collect files]** button.

The collection of the data may take several minutes. Once the log file has been created, a message appears.

2 Sending the ZIP file to the regional Metrohm representative

A ZIP file is stored on the desktop with the log files in the following format:
'OMNIS_Info_YYYYMMDD_hhmmss_mmm.zip'
YYYY = Year, **MM** = Month; **DD** = Day; **hh** = Hour; **mm** = Minute; **ss** = Second; **mmm** = Millisecond

- Send the ZIP file created on the desktop by e-mail to the regional Metrohm representative.

Running the OMNIS InfoZipper program in the program directory

1 Creating log files

- Open the Windows Explorer window.
- Open the program directory (default **...\Metrohm\OMNIS\Desktop**).
- Run the **InfoZipper.exe** program.

The collection of the data may take several minutes. Once the log file has been created, a message appears.

2 Sending the ZIP file to the regional Metrohm representative

A ZIP file is stored on the desktop with the log files in the following format:
'OMNIS_Info_YYYYMMDD_hhmmss_mmm.zip'
YYYY = Year, **MM** = Month; **DD** = Day; **hh** = Hour; **mm** = Minute; **ss** = Second; **mmm** = Millisecond

- Send the ZIP file created on the desktop by e-mail to the regional Metrohm representative.

Running the OMNIS InfoZipper program from the start menu

1 Creating log files

- Open the Windows start menu.
- Search for the **OMNIS InfoZipper** program.
- Execute the **OMNIS InfoZipper** program.

The collection of the data may take several minutes. Once the log file has been created, a message appears.

2 Sending the ZIP file to the regional Metrohm representative

A ZIP file is stored on the desktop with the log files in the following format:
'OMNIS_Info_YYYYMMDD_hhmmss_mmm.zip'
YYYY = Year, **MM** = Month; **DD** = Day; **hh** = Hour; **mm** = Minute; **ss** = Second; **mmm** = Millisecond

- Send the ZIP file created on the desktop by e-mail to the regional Metrohm representative.

No customer-specific information is stored in the log files.
You will find further information on data storage in the OMNIS Software at *OMNIS Software – Licensing process*.

See also

OMNIS Software – Faults (chapter 7.1, page 1236)

Sending OMNIS environment information (chapter 6.2, page 1235)

7.4 Collecting instrument log files

Prerequisite:

- The user has the **Manage equipment** right.

1 Opening Instrument management

- Select the affected instrument under **Equipment** ▶ **Instruments**.

The depiction of the selected instrument with its functional units is shown with a green frame.

2 Collecting instrument log files

- Click on to open the **Properties** window.
- Click on **[Collect files]** to start reading out the instrument log file under **Properties** ▶ **Licenses and firmware**.
- Wait until the **[Collect files]** button is activated once again. The reading out of the data may take several minutes.

The instrument log file is stored in the **...ProgramData\Metrohm\OMNIS\logs** directory.

The directory with the backup files is hidden by default in Windows.

If the reading out of the data or the writing of the instrument log file ends with an error message, then follow the instructions contained in the error message.

The data in the instrument log file is reset when the instrument is restarted.

Repeat the steps for all the affected instruments and then start the **OMNIS InfoZipper** program *(see "Collecting OMNIS system information", chapter 7.3, page 1238)*.

See also

OMNIS Software – Faults (chapter 7.1, page 1236)