OMNIS Software 2.17.0

Product manual

EN V-2.17.0 / 2021-09-10

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This documentation has been prepared with great care. However, errors can never be entirely ruled out. Please send comments regarding possible errors to the address above.

Disclaimer

Deficiencies arising from circumstances that are not the responsibility of Metrohm, such as improper storage or improper use, etc., are expressly excluded from the warranty. Unauthorized modifications to the product (e.g. conversions or attachments) exclude any liability on the part of the manufacturer for resulting damage and its consequences. Instructions and notes in the Metrohm product documentation must be strictly followed. Otherwise, Metrohm's liability is excluded.

Table of contents

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

NOTICE

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

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.

NOTICE

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: *User rights – Directory (see chapter 4.6.7.3, page 62)*

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

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: *Importing software help (see chapter 3.1, page 10)*.

Information packs on OMNIS hardware components can also be loaded manually into the software help (*Importing software help (see 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: *Software help – Overview – OMNIS Help (see chapter 1.4, page 5)*

Further information on the OMNIS Software

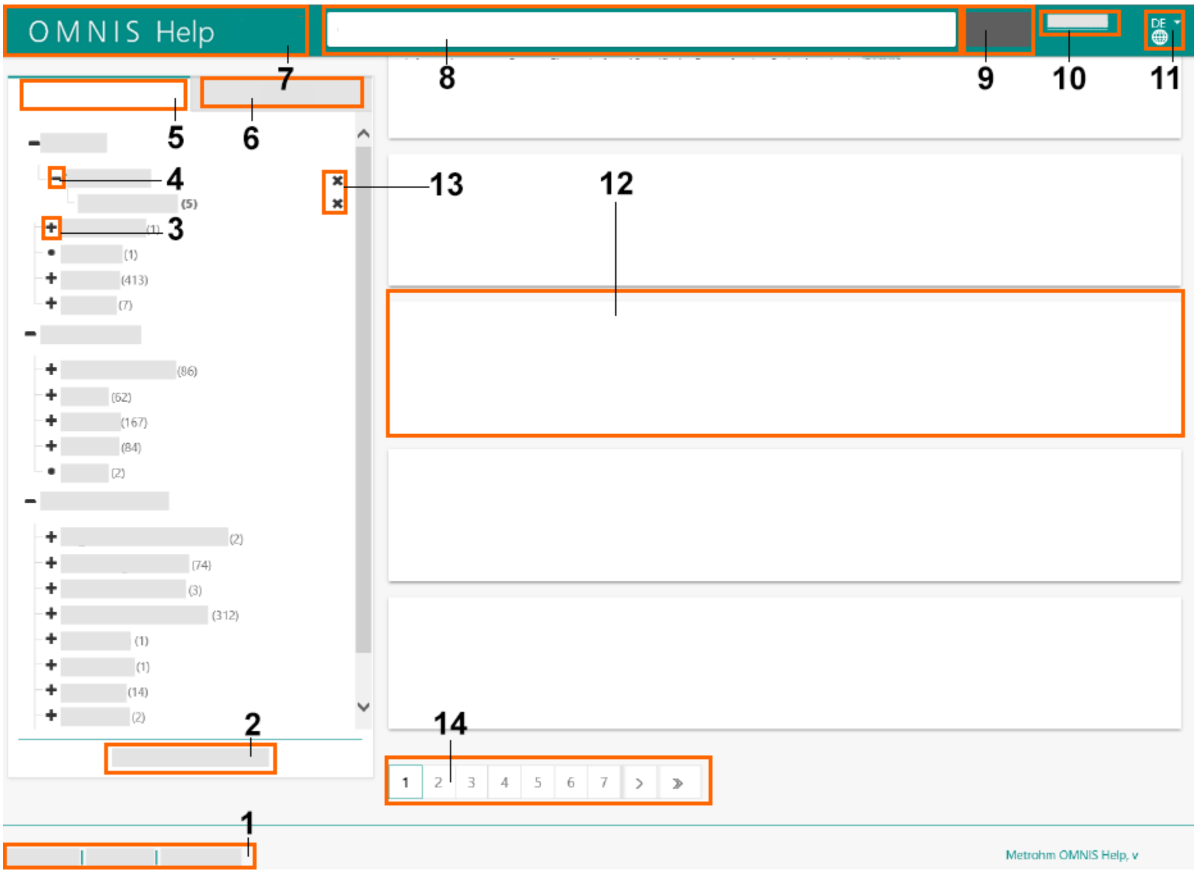
In addition to the **OMNIS Help**, which is installed locally on the computer, all information on software functions and OMNIS hardware components is available online in the Metrohm Knowledge Base *https://guide.metrohm.com/*

See also

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

Importing software help (chapter 3.1, page 10)

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.

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 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 *http://www.metrohm.com/en/support-and-service/software-center/omnis/* 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 path 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.

NOTICE

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 119)

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

- You can find the templates 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 „templates" 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

- In the **Processes** work area under **Operating procedures**, click on the icon.
  or
  In the **Processes** work area under **Methods**, click on the icon.
- The **Import method / operating procedure** dialog window opens.
- Open the folder with the unpacked templates, select the required *.opro files and click on **[Open]**.
  The contained OMNIS work systems will also be imported.
  The operating procedures and methods are imported into the OMNIS Software.

NOTICE

The templates need to be adapted to your system. You can find important information and help in the descriptions of the templates. Read the corresponding description before you import the templates *Operating procedure – Templates for titration* / *Operating procedures / methods – Templates for TitrIC flex*.

See also

Operating procedure – Definition (chapter 5.9.1, page 260)

4 Start-up

4.1 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 activated later as required. If you have questions about software licenses, contact your regional Metrohm representative.

Activating the initial software license

Prerequisite:

- The OMNIS Software is installed.
- An Internet connection is available.
- The ticket number (format: 12345-12345-ABCDE-ABCDE-1X2Y3) is available.
- The customer number (format: 123-456789) is available.

1 Starting the OMNIS Software

- Start the OMNIS Software.

A message appears.

2 Starting the licensing wizard

- Click on **[Activate license]** to start the licensing wizard.

A new window is opened.

3 Selecting the type of licensing

- Select the type of licensing **[Online licensing]** or **[Offline licensing]**.
- Follow the instructions of the licensing wizard.

NOTICE

- 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.

4 Closing the window

- When the **The license was successfully installed.** message appears, close the window by clicking on **[Exit]**.

Activating additional software licenses

Prerequisite:

- The OMNIS Software is installed.
- An Internet connection is available.
- The ticket number (format: 12345-12345-ABCDE-ABCDE-1X2Y3) is available.
- The customer number (format: 123-456789) is available.

If the user management for the OMNIS Software has been activated:

- The user has the **Activate software licenses** right.

1 Starting the OMNIS Software

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

A new window is opened.

2 Selecting the type of licensing

- Select the type of licensing **[Online licensing]** or **[Offline licensing]**.
- Follow the instructions of the licensing wizard.

NOTICE

- 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 window

- When the **The license was successfully installed.** message appears, close the window by clicking on **[Exit]**.

NOTICE

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

4.2 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.

NOTICE

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

Prerequisite:

- The OMNIS Software is installed.

- An Internet connection is available.
- The ticket number (format: 12345-12345-ABCDE-ABCDE-1X2Y3) is available.
- The customer number (format: 123-456789) is available.

1 Opening 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 Starting the licensing wizard

- Click on **[Activate functions]** to start the licensing wizard.

A new window is opened.

4 Selecting the type of licensing

- Select the type of licensing: **[Online licensing]** or **[Offline licensing]**.
- Follow the instructions of the licensing wizard.

NOTICE

- 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.

NOTICE

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

5 Closing the window

- When the **The license was successfully installed.** message appears, close the window by clicking on **[Exit]**.

The additional instrument functions are now activated.

NOTICE

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.

4.3 Setting up OMNIS Software

NOTICE

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

Select language to use

1 Select Dialog language

- Select the dialog language from the selection list in **Settings ▶ General settings**.

After restarting the OMNIS Software, the user interface is displayed in the selected dialog language.

2 Select System language

- Select the system language in the selection list in **Settings ▶ Advanced settings**.

After restarting the OMNIS Software, reports and audit trail entries are output in the selected system language and are saved *Creating a report (see chapter 5.8.1.5, page 159)*.

Show Emergency stop function

1 Show emergency stop function

- Activate the **Show emergency stop function** function by clicking on the check box in **Settings ▶ General settings**.

The STOP icon is shown on the user interface at the front.

NOTICE

The emergency stop function is intended for an emergency.

When the STOP button is pressed, all functional units stop and current determinations are canceled immediately without carrying out the optional run **Execute on stop**. With the software, the functional units can be subsequently moved to a safe status and reinitialized. The emergency stop function can be moved around the screen as required.

See also

Audit trail work area – Actions (chapter 5.12, page 917)

Modification comment – Brief description (chapter 5.5, page 131)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

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Setting up a printer (chapter 5.13.1, page 932)

Locking conformity (chapter 4.4, page 19)

Signature – Brief description (chapter 5.6, page 131)

4.4 Locking conformity

NOTICE

The functions for **ComplianceFDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** are shown if the following conditions have been met:

- A valid Software license (**Compliance/Regulation Stand-Alone**) is used.
- User management is activated.
- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

Once conformity 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 conformity

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.

NOTICE

If the audit trail is activated, all the modifications made in the OMNIS Software are recorded.

2 Activating signatures

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

NOTICE

Signatures allow for a two-step release 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.

NOTICE

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

4 Locking conformity

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

A dialog is opened.

5 Confirm the message

NOTICE

Once conformity 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.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

User management settings – Brief description (chapter 4.6.4, page 43)

Setting up OMNIS Software (chapter 4.3, page 17)

Audit trail work area – Actions (chapter 5.12, page 917)

Modification comment – Brief description (chapter 5.5, page 131)

Signature – Brief description (chapter 5.6, page 131)

4.5 User management (Active Directory) – Actions

The following actions can be carried out in the **User management** work area in the subsections using the **User management with Active Directory integration**:

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

- All users can be viewed 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 recorded user groups can be viewed 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.

- New user roles can be created, all existing user roles can be managed, and user roles can be 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

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

User rights – Directory (chapter 4.6.7.3, page 62)

Managing passwords (chapter 4.6.8, page 68)

Activating user management (Active Directory) (chapter 4.6.2, page 25)
Activating user management (Active Directory) (chapter 4.6.2, page 25)

Activating user management (OMNIS) (chapter 4.6.3, page 39)

4.6 User management (OMNIS) – Actions

The following actions can be carried out in the **User management** work area in the subsections using the **OMNIS-local user management without Active Directory integration**:

- 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 can be managed and users can be assigned to user groups in **User management ▶ User list**.
- New user groups can be created, all existing user groups can be managed, and user groups with user roles can be linked in **User management ▶ User groups**.
- New user roles can be created, all existing user roles can be managed, and user roles can be 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

Managing passwords (chapter 4.6.8, page 68)

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

User rights – Directory (chapter 4.6.7.3, page 62)

Managing passwords (chapter 4.6.8, page 68)

4.6.1 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 link 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 to user groups remains within the OMNIS Software.

NOTICE

There are two possible ways to set up user management with Active Directory integration: Either initially at the time user management is set up, or retroactively to the local user management (OMNIS), if this has already been activated and is in use.

- **User management (OMNIS):** This is an internal user management which is integrated locally 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.

See also

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User groups – Definition (chapter 4.6.6, page 55)

User roles – Definition (chapter 4.6.7, page 59)

User rights – Directory (chapter 4.6.7.3, page 62)

Activating user management (Active Directory) (chapter 4.6.2, page 25)
Activating user management (Active Directory) (chapter 4.6.2, page 25)

Activating user management (OMNIS) (chapter 4.6.3, page 39)

4.6.2 Activating user management (Active Directory)

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 user groups can 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:

- *(see "Option 1", page 26)* To begin with when setting up user management.
- *(see "Option 2", page 32)* By setting up the Active Directory integration after activating the local user management (OMNIS).

NOTICE

The Active Directory integration cannot be deactivated again for traceability reasons.

In both cases, successful setup depends on the specification of **Domain**, **User name**, **Password** and **Synchronization group** or **Distinguished Name** 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: *(see "Modifying the connection settings", page 36)*

Option 1

1 Searching the Distinguished Name in the LDAP browser and copying it

- Open the **LDAP browser** program (e.g. by Softerra).

> **NOTICE**
>
> The correct node must be selected in the area window. The value of the **object class** (**2**) must be **group**. The **DN (Distinguished Name)** node is in the same tree.

- Select the **DN (Distinguished Name)** (**1**).
- Copy the path.

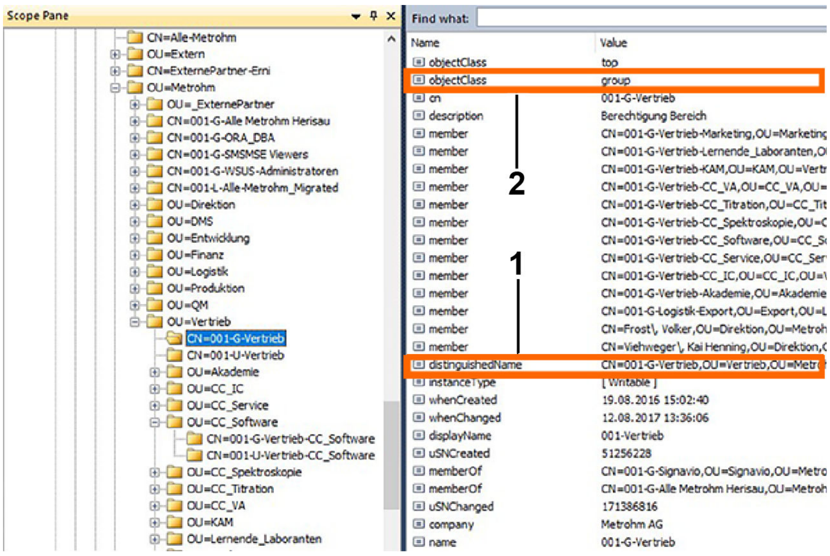


Figure 1 Example for an LDAP browser

2 Opening the OMNIS Software

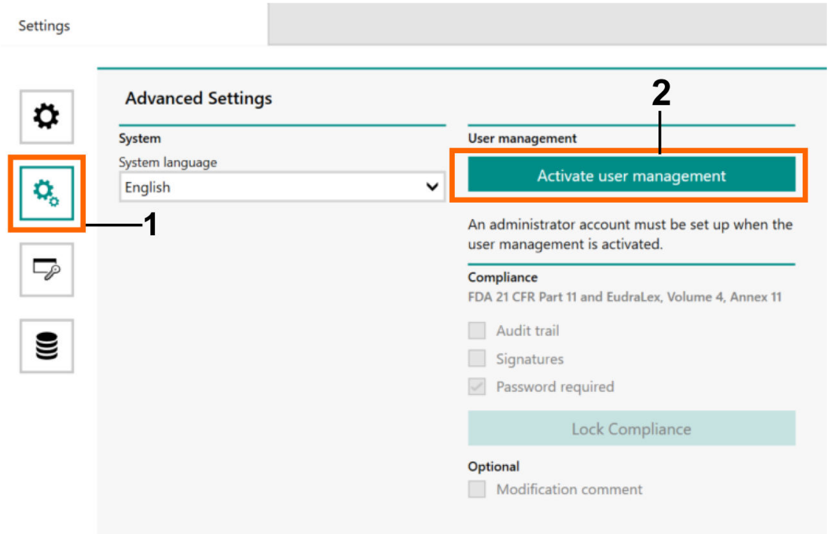
- Open the OMNIS Software.

3 Activating user management

NOTICE

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

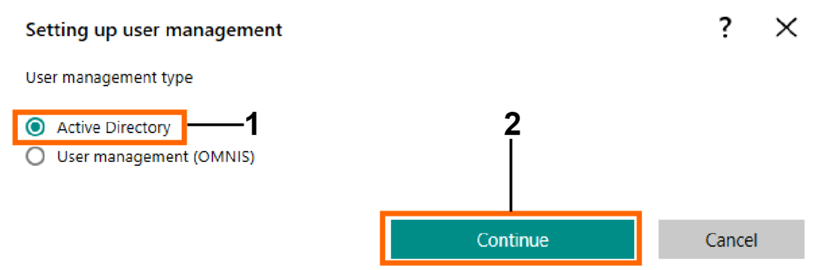
- In **Settings ▶ Advanced settings ▶ User management** (**1**), click on **[Activate user management]** (**2**).



A dialog is opened.

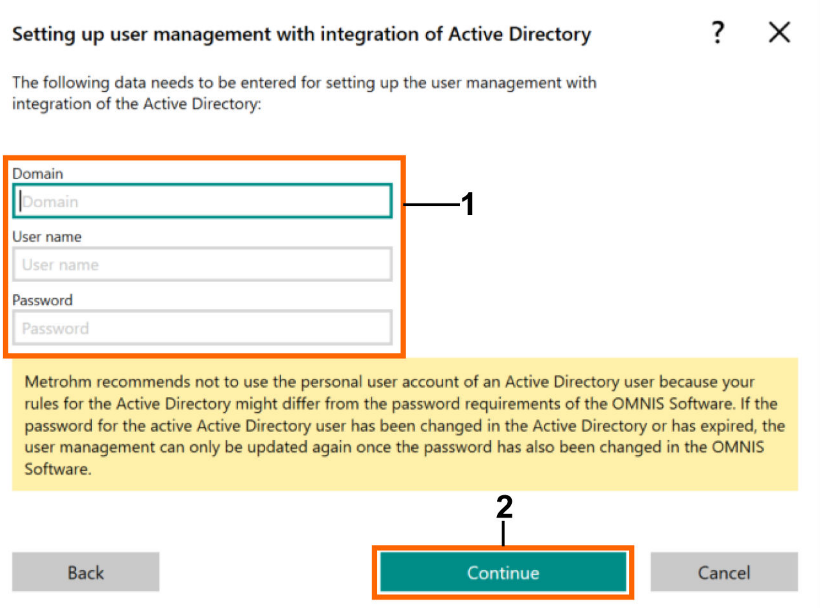
4 Selecting the user management type

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



5 Entering domain, user name and password

- Enter **Domain**, **User name** and **Password** (**1**).
- Click on **[Continue]** (**2**) to continue the setup.



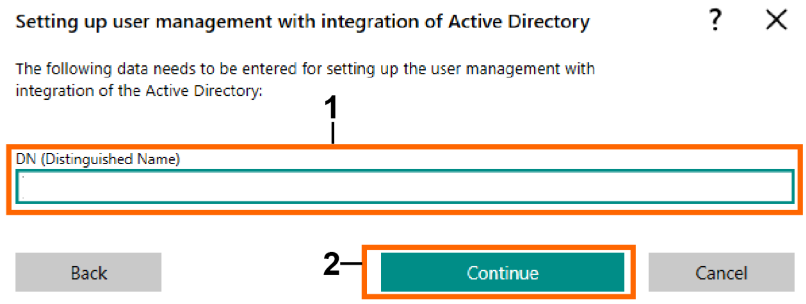
NOTICE

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 your rules for the Active Directory might differ from the password requirements of the OMNIS Software. If the password for the used Active Directory user has been changed in the Active Directory or has expired, the user management can no longer be updated until the password has also been changed in the OMNIS Software.

6 Entering the synchronization group

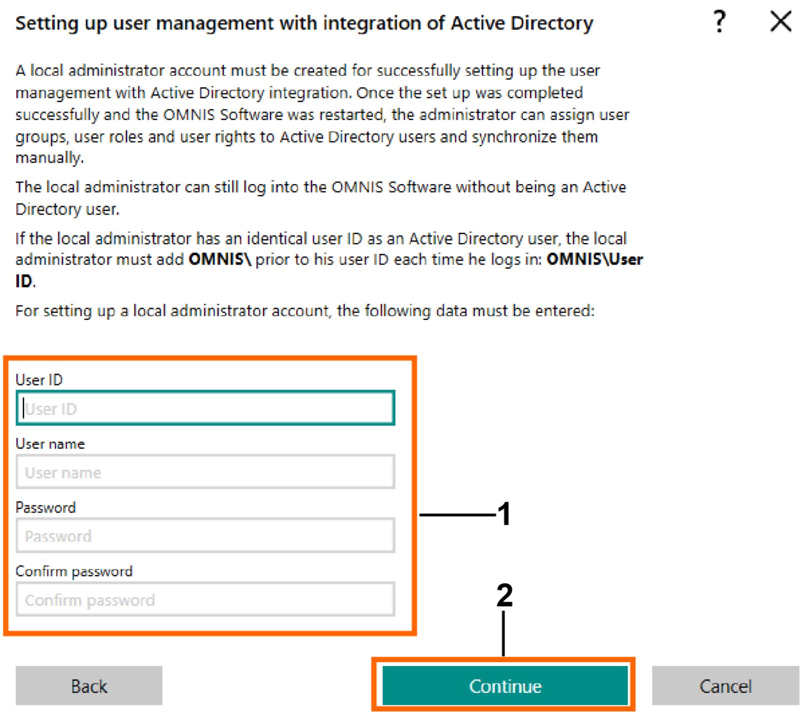
- Enter the entire **DN (Distinguished Name)** (**1**).
- Click on **[Continue]** (**2**) to continue the setup.



> **NOTICE**
>
> The selected synchronization group *(see figure 1, page 26)* must be the **parent group**. All subsequently assigned groups *(see figure 1, page 26)* must be added as subgroups **childs** of the selected synchronization group.

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.



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.

NOTICE

If the local administrator has the same user ID as an Active Directory user, then the local 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 local administrator.

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

10 Opening a user group

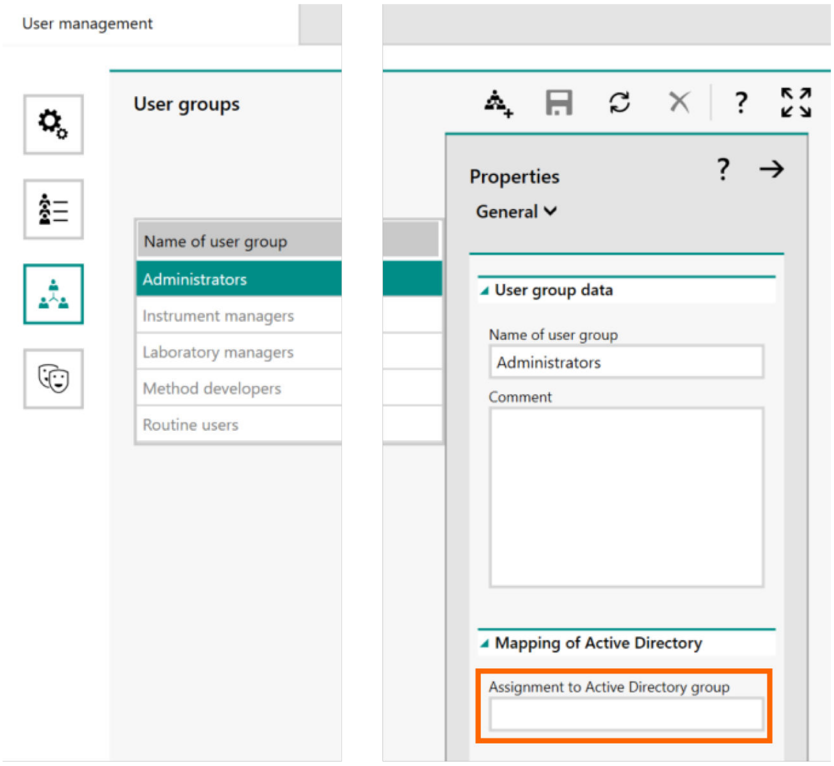
- Select a user group in **User management ▶ User groups** or create a new user group by clicking on .
- Open the settings for the selected or newly created user group by clicking on .

11 Searching a user group

- Search in the **LDAP browser** for the user group to be connected *(see "Option 1", page 26)*.

12 Assignment to Active Directory group

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

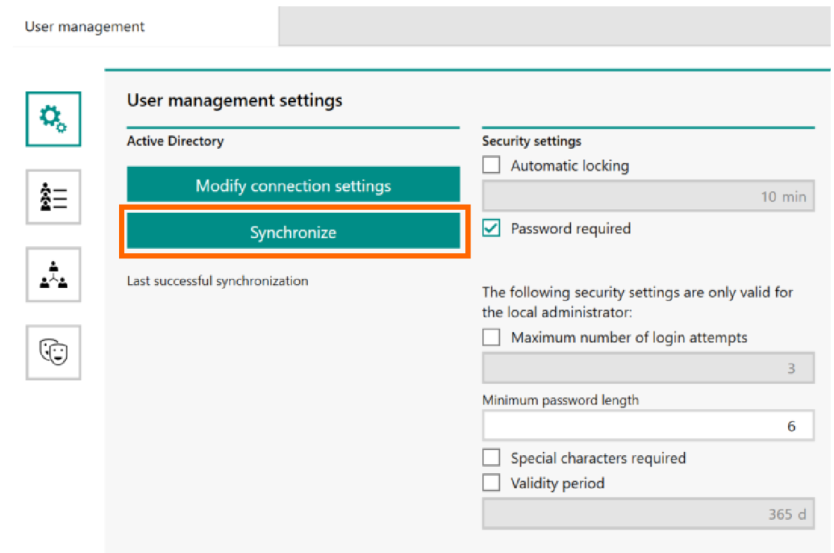


13 Saving changes

- Click on to save the data entered.

14 Synchronizing user management settings

- 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**.

NOTICE

Repeat steps 8 to 14 for all the relevant user groups. The OMNIS Software can then be used with the settings used in the Active Directory.

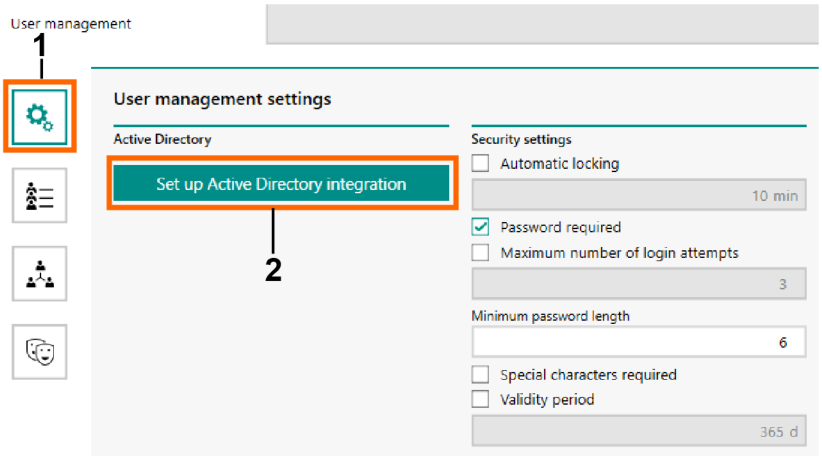
Option 2

Prerequisite:

- User management (OMNIS) is activated.
- Steps 1 to 3 have been executed *(see "Option 1", page 26)*.

1 Retroactive integration of Active Directory

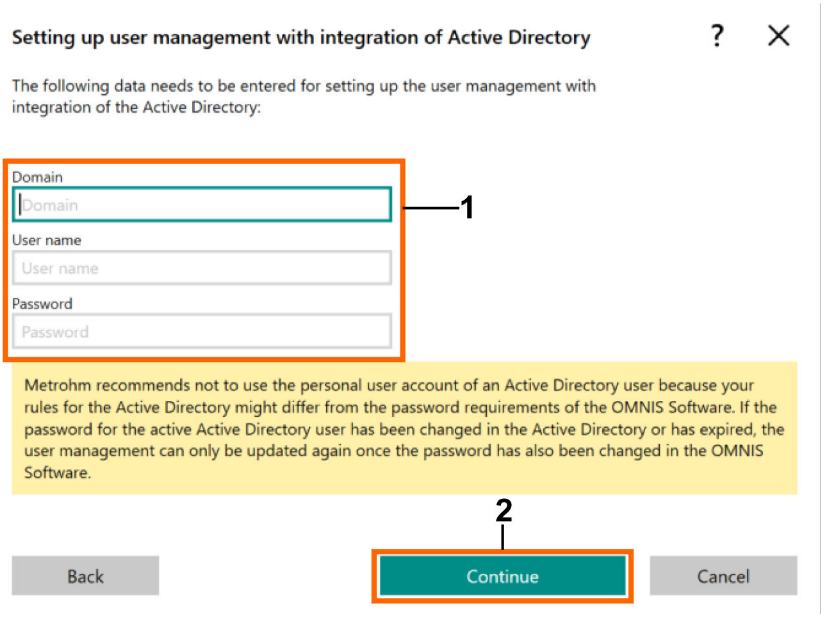
- In **User management ▶ User management settings** (**1**), click on **[Set up Active Directory integration]** (**2**).



A dialog is opened.

2 Entering domain, user name and password

- Enter the **Domain**, **User name** and **Password** (**1**).
- Click on **[Continue]** (**2**) to continue the setup.

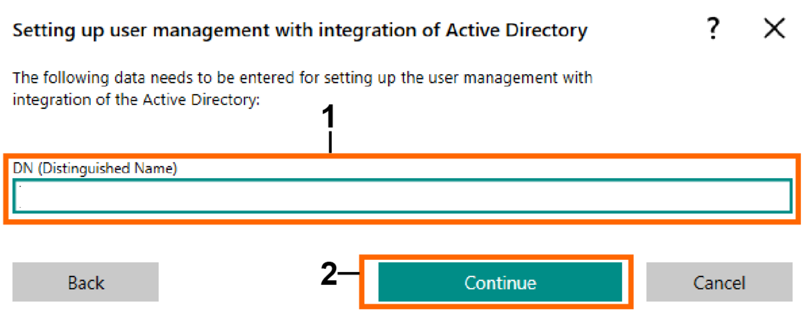


NOTICE

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

3 Entering the synchronization group

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



NOTICE

The selected synchronization group *(see figure 1, page 26)* must be the **parent group**. All subsequently assigned groups *(see figure 1, page 26)* must be added as subgroups **childs** of the selected synchronization group.

4 Confirming the setup

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

5 Restarting the OMNIS Software

- Start the OMNIS Software as an administrator.

NOTICE

If the local administrator has the same user ID as an Active Directory user, then the local 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 local administrator.

All users except the administrator that was last created are deactivated in the local user management, if the local user management of the OMNIS Software was previously used. New user accounts must be created exclusively through Active Directory.

6 Opening a user group

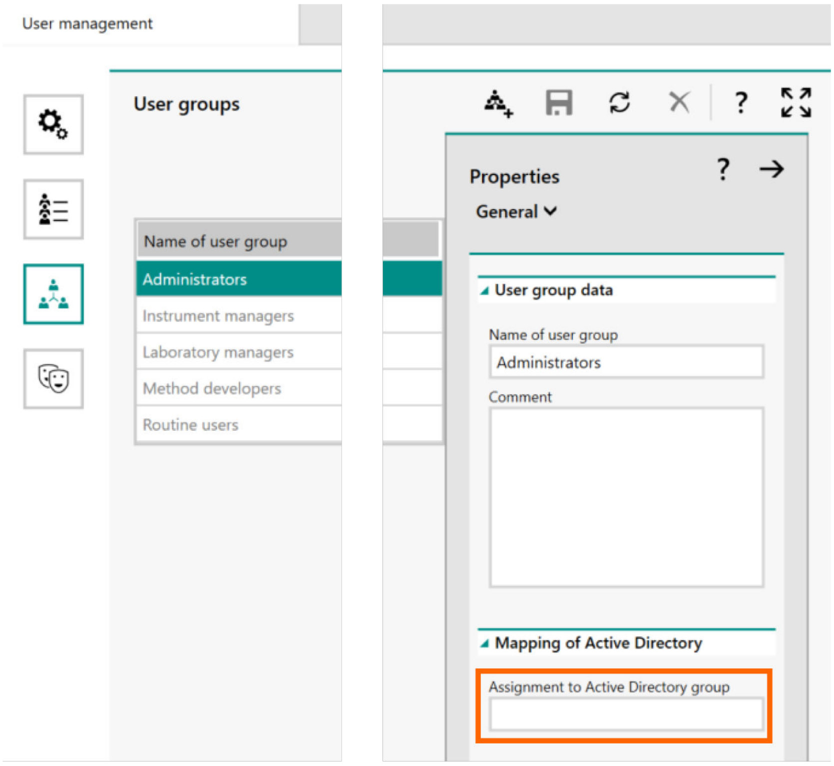
- Select a user group in **User management ▶ User groups** or create a new user group by clicking on .
- Open the settings for the selected or newly created user group by clicking on .

7 Searching a user group

- Search in the **LDAP browser** for the user group to be connected *(see figure 1, page 26)*.

8 Assignment to Active Directory group

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

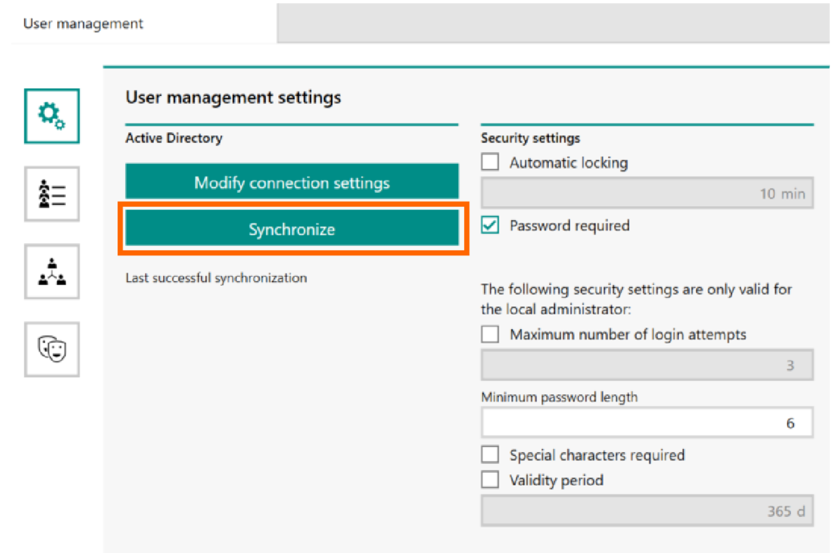


9 Saving changes

- Click on  to save the data entered.

10 Synchronizing user management settings

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



11 Updating a user list

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

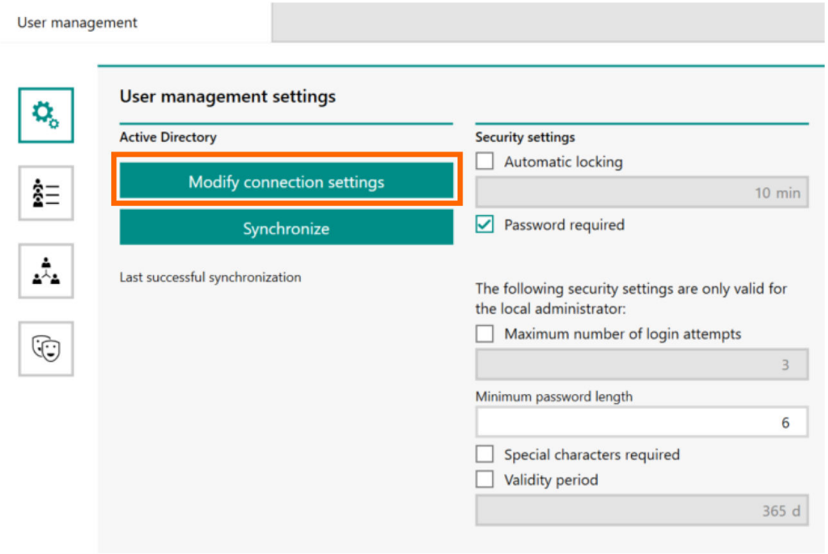
Modifying the connection settings

Prerequisite:

- User management with Active Directory integration is activated.

1 Modifying data

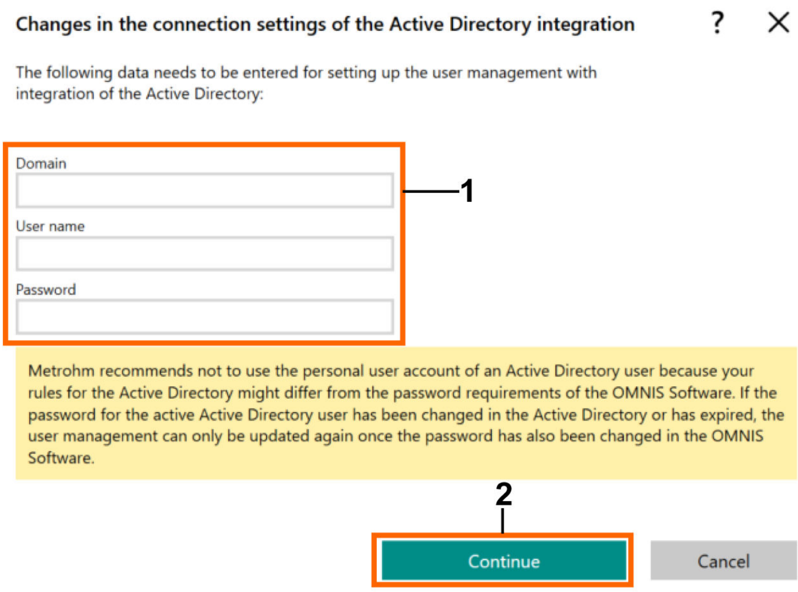
- Click on **[Modify connection settings]** in **User management ▶ User management settings** to change the entered data of the Active Directory integration.



A dialog with pre-filled input fields opens.

2 Entering domain, user name and password again

- Enter the **Domain**, **User name** and **Password** again, if necessary (**1**).
- Click on **[Continue]** to continue changing the data (**2**).



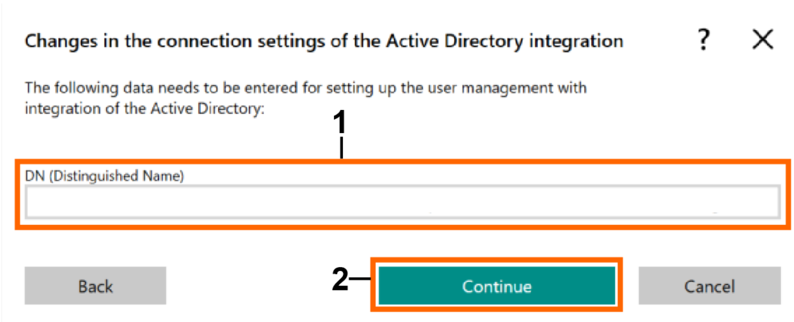
NOTICE

Metrohm does not recommend using the personal user account of an Active Directory user because your rules for the Active Directory might differ from the password requirements of the OMNIS Software. If the password for the used Active Directory user has been changed in the Active Directory or has expired, 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 synchronization group again

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



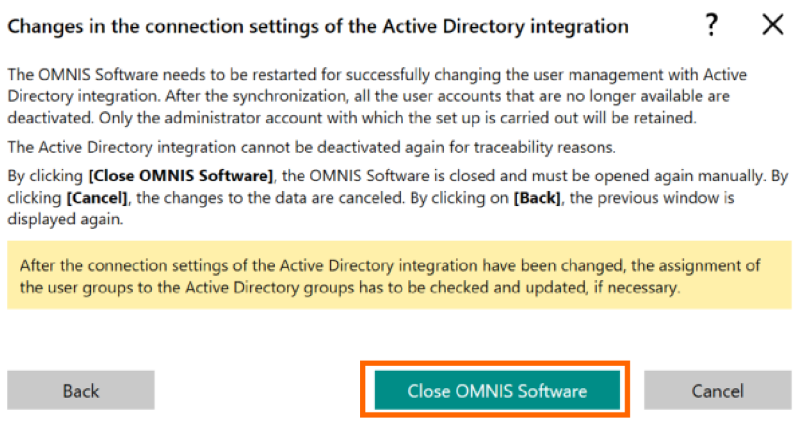
NOTICE

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]**.



NOTICE

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.

See also

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User groups – Definition (chapter 4.6.6, page 55)

User roles – Definition (chapter 4.6.7, page 59)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

Managing passwords (chapter 4.6.8, page 68)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

4.6.3 Activating user management (OMNIS)

User management (OMNIS) 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 a local administrator. The local administrator also assigns the necessary rights.

1 Activating user management (OMNIS)

NOTICE

If there are unsaved changes or running determinations, the user management cannot be activated. 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.

NOTICE

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

The new settings will not take effect until after a restart.

If the user management with Active Directory integration is activated retroactively and if the local administrator has the same user ID as an Active Directory user, then the local 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 local 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.

NOTICE

The new settings will not take effect until after a restart.

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.

The local 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.

NOTICE

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, the local 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.
- Activate the **[Reset password]** check box.
- Define a new password and confirm it with a second entry.
- Click on to save the data entered.

NOTICE

Only users with administrator rights can reset passwords.

If the local 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.

More information on password administration: *Managing passwords (see chapter 4.6.8, page 68)*

NOTICE

If the **Audit trail** function in the **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** option is switched on, then all of the changes made in the Audit trail will be recorded and listed. For more information regarding the recording of entries in the audit trail, see: *Audit trail – Directory (see chapter 5.12.1, page 917)*

See also

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User groups – Definition (chapter 4.6.6, page 55)

User roles – Definition (chapter 4.6.7, page 59)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

Managing passwords (chapter 4.6.8, page 68)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

4.6.4 User management settings – Brief description

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 to the local user management (OMNIS) by clicking on **[Set up Active Directory integration]**, if this has already been activated.

NOTICE

More information on setting up user management with or without Active Directory integration, see: *Activating user management (Active Directory) (see chapter 4.6.2, page 25)*
Activating user management (Active Directory) (see chapter 4.6.2, page 25)

Activating user management (OMNIS) (see chapter 4.6.3, page 39)

NOTICE

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 the local 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 execute 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.

If the **User management with Active Directory integration** is used, the entered data of the Active Directory integration can be changed by clicking on **[Modify connection settings]**. After the synchronization, all the user accounts that are no longer available are deactivated. The synchronization can be started manually and at any time by clicking on **[Synchronize]**. Date and time of the last successful synchronization are displayed here. Automatic synchronization takes place every 12 hours and after each time the Metrohm Miami LabLogic service starts.

Security settings

NOTICE

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

The following settings are available for selection:

Automatic locking	If this check box is activated, then the time in minutes until the OMNIS Software is locked automatically after the last user action (operation of the keyboard or the mouse) can be defined.
Password required	If this check box is activated, then users must enter a password when logging in. If compliance is locked in **Settings ▶ Advanced settings**, the **Password required** check box can no longer be activated or deactivated.
Maximum number of login attempts	If this check box is activated, then the maximum number of login attempts can be defined. The user is deactivated if this is exceeded. An administrator must reactivate the user.
Minimum password length	If the **Password required** check box is activated, a **Minimum password length** can be defined to increase safety.
Special characters required	If this check box is activated, the password must also contain special characters.
Validity period	If this check box is activated, an expiry time in days can be defined, after which the password must be replaced by a new one. A message is displayed that prompts the user to change his or her password.

NOTICE

In the event of activated user management with Active Directory integration, some specifications regarding security settings are applied only to the local administrator. The **Automatic locking** and **Password required** settings apply for all users.

Active Directory passwords are managed in Active Directory and cannot be changed in the OMNIS Software. Further information on password administration: *Managing passwords (see chapter 4.6.8, page 68)*

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

All settings and changes are saved by clicking on , after which they also become effective.

NOTICE

If the **Audit trail** function in the **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** option is switched on, 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: *Audit trail – Directory (see chapter 5.12.1, page 917)*

See also

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

Managing passwords (chapter 4.6.8, page 68)

Locking conformity (chapter 4.4, page 19)

User rights – Directory (chapter 4.6.7.3, page 62)

4.6.5 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 **local user management (OMNIS)**.

NOTICE

For traceability reasons, existing users cannot be deleted again.

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

NOTICE

New users can no longer be created and edited after activation of the user management with Active Directory integration. All previously existing user accounts are deactivated after the successful setting up of the user management with Active Directory. 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**.

If the local 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 Metrohm representative should be contacted in such cases. Additional information on password administration: *Managing passwords (see chapter 4.6.8, page 68)*

Overview list

The following data of all users is shown 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 local OMNIS user that can be changed in the properties.
User group	Name of the user group which contains one or more users.
User roles	User roles which were assigned to the user groups.
Last login	Date and time of the last login.

See also

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

Managing passwords (chapter 4.6.8, page 68)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

4.6.5.1 User list – Properties

Clicking on  in **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

NOTICE

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

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

<table>
<tr><td>User ID</td><td>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.</td></tr>
<tr><td>User name</td><td>Entry of the mandatory data user name. The user name must consist of the first name and last name and can be retrospectively changed.</td></tr>
<tr><td>E-mail address</td><td>Entry of user's e-mail address. The entry is optional and can be changed retrospectively.</td></tr>
<tr><td>Object ID</td><td>Object ID of user is displayed. The user is clearly identified with the object ID and the user ID.</td></tr>
<tr><td>User status</td><td>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.</td></tr>
<tr><td>Reset password</td><td>The administrator can reset a user's password using a check box.</td></tr>
<tr><td>Comment</td><td>Enter comments about the user. A maximum of 255 characters are allowed in the comment field.</td></tr>
</table>

User groups

In this subsection, the OMNIS user or Active Directory user can be assigned to 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 predefined user groups are available:

- **Administrators**
  The **Administrators** user group is assigned the **Administrator** user role. With this assignment, the user group receives the rights of the **Administrator** user role.

- **Instrument managers**
  The **Instrument managers** user group is assigned the **Instrument manager** user role. With this assignment, the user group receives the rights of the **Instrument manager** role.
- **Laboratory managers**
  The **Laboratory managers** user group is assigned the **Lab manager** user role. With this assignment, the user group receives the rights of the **Laboratory manager** user role.
- **Method developers**
  The **Method developers** user group is assigned the **Method developer** user role. With this assignment, the user group receives the rights of the **Method developer** user role.
- **Routine users**
  The **Routine users** user group is assigned the **Routine user** user role. With this assignment, the user group receives the rights of the **Routine user** user role. If a new user is created, then they are automatically assigned the **Routine user** user group. This assignment can be changed.

See also

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

Managing passwords (chapter 4.6.8, page 68)

Locking conformity (chapter 4.4, page 19)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

4.6.5.2 Managing users

To create new users, the user management (OMNIS) must be activated and a local administrator account must be set up first. Once the set up of the user management was completed successfully and the OMNIS Software was restarted, the local administrator can log into the OMNIS Software and then create other local users.

1 Activating user management (OMNIS)

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

NOTICE

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

NOTICE

- The User ID must be unique and may not contain any of the following special characters: Λ?*%;'":|[]+=<>,. 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 local 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.

NOTICE

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).
- Click on to save the data entered.

NOTICE

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

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

NOTICE

The user registered is automatically a member of the **Routine users** user group.

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 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

Activating user management (Active Directory) (chapter 4.6.2, page 25)
Activating user management (Active Directory) (chapter 4.6.2, page 25)

Activating user management (OMNIS) (chapter 4.6.3, page 39)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

4.6.5.3 User login

The user is given a password by the administrator for initial 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 log-in data

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

NOTICE

Passwords of Active Directory users must be changed directly in Active Directory.

More information on password administration: *Managing passwords (see chapter 4.6.8, page 68)*

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.

NOTICE

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

At the time of the first login, the user must define his or her future password in the **Change password** dialog which appears automatically.

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 deactivated.

NOTICE

If the **Audit trail** function in the **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** option is switched on, 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: *Audit trail – Directory (see chapter 5.12.1, page 917)*

See also

Managing passwords (chapter 4.6.8, page 68)

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User groups – Definition (chapter 4.6.6, page 55)

User roles – Definition (chapter 4.6.7, page 59)

User rights – Directory (chapter 4.6.7.3, page 62)

Activating user management (Active Directory) (chapter 4.6.2, page 25)
Activating user management (Active Directory) (chapter 4.6.2, page 25)

Activating user management (OMNIS) (chapter 4.6.3, page 39)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Locking or unlocking OMNIS Software (chapter 5.4, page 129)

Locking conformity (chapter 4.4, page 19)

4.6.6 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 **local user management (OMNIS)**.

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.

Overview list

The following data for all user groups is displayed in the overview list:

Name of user group	Name of user group.
Active Directory group	Name of the assigned Active Directory group.
Number of members	Number of active and inactive members.
Created	Date and time the user group was created.

NOTICE

In the event of user management with Active Directory integration, an additional column **Active Directory group** exists after completed synchronization.

See also

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

4.6.6.1 User groups – Properties

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

General

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

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

NOTICE

The mapping by the local administrator is additionally carried out in this subsection through the use of the user management with Active Directory integration. 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 an object in the Active Directory. This object contains multiple Active Directory users who are to be assigned to the selected user group and who are thus to receive 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.

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.

NOTICE

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.

NOTICE

Using the 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 thereby 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:*User roles – Directory (see chapter 4.6.7.2, page 61)*

See also

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

4.6.6.2 User groups – Directory

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.

See also

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

4.6.7 User roles – Definition

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

Overview list

The following data from all user roles is shown in the overview list:

Name of the user role	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

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

4.6.7.1 User roles – Properties

Clicking on in **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 to the user role in this subsection:

Name of the user role	Enter required 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

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Directory (chapter 4.6.7.2, page 61)

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

4.6.7.2 User roles – Directory

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 a user group and is only provided for work by Metrohm Service. The trained and certified Metrohm Service engineer can login to the OMNIS Software using a dongle to carry out service work.
- **Instrument manager**: The Instrument manager user role contains all the necessary rights for maintenance of laboratory devices and accessories.
- **Laboratory managers**: The Laboratory manager user role includes all rights for the **Samples**, **Processes**, **Equipment** and **Audit trail** work areas to be able to perform tasks in these areas.
- **Method developer**: The Method developer user role includes the rights to record methods and operating procedures, to sign methods and operating procedures at level 1 as well as to have limited access to the Samples work area.
- **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.

See also

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User list – Properties (chapter 4.6.5.1, page 47)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Directory (chapter 4.6.6.2, page 58)

User roles – Definition (chapter 4.6.7, page 59)

User roles – Properties (chapter 4.6.7.1, page 60)

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management – Definition (chapter 4.6.1, page 24)

User rights – Directory (chapter 4.6.7.3, page 62)

4.6.7.3 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.

> **NOTICE**
>
> 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 only take effect after a restart of the OMNIS Software.
>
> Contact the internal IT administrator in the event of missing rights.

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 activated, the **Manage samples** and **Manage sample lists** right is automatically also assigned.
Manage sample lists	▪ Show sample lists.
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.
Delete sample lists	▪ Open sample lists, rename and save them. ▪ 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. ▪ 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	▪ Adding sample data in the sample list.
Edit samples/not analyzed sub-samples	▪ Open sample lists, rename and save them. ▪ Edit sample data and subsample data from sub-samples 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 and paste samples and subsamples from a sample list.
Delete sam-ples/subsam-ples	▪ Open sample lists, rename and save them. ▪ Delete selected samples and subsamples perma-nently from the sample list (the samples and sub-samples can have any status when deleting).
Import sam-ples	▪ Open sample lists, rename and save them. ▪ Import CSV files and OSIN files manually.
Export sam-ples	▪ Open sample lists, rename and save them. ▪ Export samples, associated subsamples and deter-mination data. ▪ The **Manage search queries** right is also required to export samples, associated subsam-ples 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 pre-vented. ▪ 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	**Unreleased operating procedures** are operating procedures without Level 2 signature. Operating procedures are considered released as soon as they are signed at Level 2. ▪ Open sample lists, rename and save them. ▪ Start or stop determinations. ▪ Select the type of the determinations.
Start determinations with released operating procedures	**Released operating procedures** are operating procedures with Level 2 signature. ▪ Open sample lists, rename and save them. ▪ Start or stop determinations. ▪ Select the type of the determinations.
Reprocess subsamples	▪ Change the evaluation of the analysis. ▪ Recalculate results. ▪ Modifying 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.
Reset subsamples to status "Ready"	▪ Reset the subsamples to the "Ready" status.
Create reports manually	▪ Create reports.
Manage search queries	▪ Create, edit, rename, save and delete 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	▪ Open the list of sample profiles. ▪ Open the sample profile. ▪ Create, edit, save and delete sample profiles.

Samples	Permission for the following actions
Manage system variables	▪ Open the list of system variables. ▪ Create, edit, save and 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.

Processes	Permission for the following actions
Manage processes	▪ View overview list of operating procedures and methods. ▪ Create, open, edit, save, duplicate, import, export and delete operating procedures and methods. ▪ Restore operating procedures and methods from analyzed subsamples.
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.

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. Once a lower-level right is activated, the permission for this right is automatically activated as well.
Manage instruments	▪ Reserve instruments and release them once again. ▪ Edit instrument properties.
Operate instruments manually	▪ Display instruments. ▪ Execute functions of instruments and functional units.
Manage work systems	▪ View the overview list of the work systems. ▪ Create, edit, save and delete work systems.
Control work systems	▪ Open and stop the work system.

Equipment	Permission for the following actions
Manage sensors	▪ Open the list of sensors. ▪ Add, save and delete the sensor. ▪ Edit the properties of the sensor. ▪ Define the advance warning time.
Manage solutions	▪ Open the list of solutions. ▪ Add, save and delete the solution. ▪ Edit the properties of the solution.
Manage sample racks	▪ Open the list of sample racks. ▪ Save and delete sample racks. ▪ Edit the properties of the sample rack.
Manage calibration buffers	▪ Create, edit, save and delete tables of calibration buffers. ▪ Delete calibration buffers.
Manage standards	▪ Open the list of standards. ▪ Import and delete standards. ▪ Edit the properties of the standard.

Models	Permission for the following actions
Manage models	The right permits general access to the models. Additional differentiated lower-level rights for models can be assigned. Once a lower-level right is activated, the permission for this right is automatically activated as well.
Manage prediction models	▪ Open the list of prediction models. ▪ Show, create, edit and publish prediction models. ▪ Import and export prediction models.
Manage slope/y-intercept corrections	▪ Open the list of slope/y-intercept corrections. ▪ Show, create and publish slope/y-intercept corrections. ▪ Import and export slope/y-intercept corrections.

Audit Trail	Permission for the following actions
Show audit trail	▪ Open and filter the audit trail.
Export audit trail	▪ Export the audit trail in a CSV file.
Archive audit trail	▪ Archive audit trail.

User management	Permission for the following actions
Manage users	▪ Create, edit and deactivate or activate 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.

Settings	Permission for the following actions
Manage settings	The right permits general access to the system settings. Additional differentiated lower-level rights for settings can be assigned. Once a lower-level right is activated, the permission for this right is automatically activated as well.
Manage general settings	▪ Edit all general settings (dialog languages, emergency stop function). ▪ Edit print settings. ▪ Edit notifications.
Manage advanced settings	▪ Edit all advanced settings (system languages). ▪ Activate user management. ▪ Edit the conformity settings.
Activate software licenses	▪ Add software licenses.
Show data management	▪ Access to data management with display of the occupied or free storage capacity of the database. ▪ View connection settings of the external database. ▪ Back up the local database manually and automatically.

See also

User roles – Directory (chapter 4.6.7.2, page 61)

User roles – Properties (chapter 4.6.7.1, page 60)

User groups – Definition (chapter 4.6.6, page 55)

User groups – Properties (chapter 4.6.6.1, page 56)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

User list – Definition (chapter 4.6.5, page 46)

4.6.8 Managing passwords

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 a password

- Enter a new password in the **Change password** window and save it by clicking on **[Change password]**.

NOTICE

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 deactivated.

If users in specific roles people 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 User

- Users must consult the administrator for resetting their password.

2 Active Directory users

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

NOTICE

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 local administrator can change his or her password in the OMNIS Software. Passwords of Active Directory users are only changed and managed in Active Directory.

3 Local administrator

- The local administrator cannot reset the password on his own.
- If the local administrator has previously furnished one or more Active Directory users with the **Manage users** right, then the local 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 local administrator.

NOTICE

Metrohm recommends defining at least one other local administrator in the OMNIS Software who comes from the Active Directory. The local IT administrator also has the option of contacting the regional Metrohm representative.

NOTICE

If the **Audit trail** function in the **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** option is switched on, 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: *Audit trail – Directory (see chapter 5.12.1, page 917)*

See also

User interface OMNIS Software – Overview (chapter 5.2, page 92)

User management – Definition (chapter 4.6.1, page 24)

Activating user management (Active Directory) (chapter 4.6.2, page 25)

Activating user management (Active Directory) (chapter 4.6.2, page 25)

Activating user management (OMNIS) (chapter 4.6.3, page 39)

User management settings – Brief description (chapter 4.6.4, page 43)

User list – Definition (chapter 4.6.5, page 46)

User groups – Definition (chapter 4.6.6, page 55)

User roles – Definition (chapter 4.6.7, page 59)

User rights – Directory (chapter 4.6.7.3, page 62)

Locking conformity (chapter 4.4, page 19)

4.7 Database – Definition

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

NOTICE

All the details about the database can be found in the OMNIS Software under **Settings ▶ Data management** or on the **Overview** tab in the **OMNIS Database Administration** program.

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 on a dedicated Microsoft SQL Server (*Installing the OMNIS Software*).

- **OMNIS stand-alone with local database:** If this option is chosen, a 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.

NOTICE

The change to an external database on a dedicated Microsoft SQL Server can be done on the **Overview** tab in the **OMNIS Database Administration** program.

Instructions for preparing the external database for use in the OMNIS Software: *Preparing the database*

Instructions on transferring a local database that is already in use to a dedicated database server: *Transferring the database*

- **OMNIS stand-alone with a connection to an external database:** If this option is chosen, no local setup of a database is necessary, but a connection to an **external database on a dedicated Microsoft SQL Server** needs to be set up. 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 only available for a user with the necessary access rights.

NOTICE

Information on the supported versions of the Microsoft SQL Server: *Database server*

Once the external database is set up, changing to the local database **Microsoft SQL Server Express** is no longer possible.

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

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Updating the database (chapter 6.1.1, page 937)

Setting up a database (chapter 4.7.1, page 72)

Backing up the database (chapter 6.1.2, page 940)

Restoring the database (chapter 6.1.3, page 945)

Resetting the database (chapter 6.1.4, page 946)

OMNIS Database Administration – Actions (chapter 6.1, page 936)

4.7.1 Setting up a database

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)**:

- *(see "Setting up a connection to an external database on a dedicated Microsoft SQL Server", page 72)* If the external database **(dedicated Microsoft SQL Server)** is selected, an empty database first has to be set up on a dedicated database server for the OMNIS Software. Once the setup of the external database is completed, it is no longer possible to switch to the local database.
- *(see "Switching from a local to an external database", page 75)* If the local database is selected, no further setup steps are necessary. The local database **Microsoft SQL Server Express** is set up on the computer on initial installation of the OMNIS Software. It is possible to change from a local to an external database at a later time.

The connection settings can be changed after setup:

- *(see "Modifying the connection settings", page 78)* After setting up the external database, the connection settings can be changed retroactively at any time.

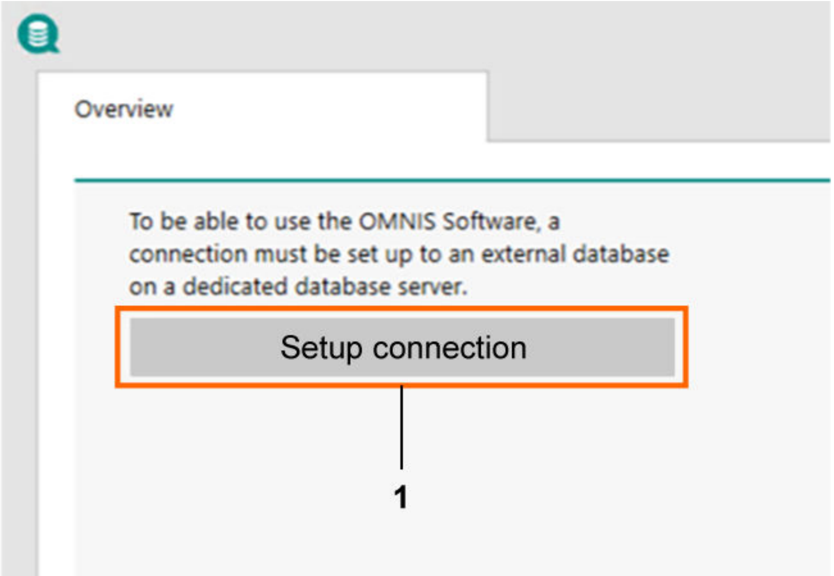
Setting up a connection to an external database on a dedicated Microsoft SQL Server

Prerequisite:

- The Windows user currently logged on has the local administrator rights.
- The **Dedicated Microsoft SQL Server** option was selected on initial installation of the OMNIS Software.
- The **OMNIS Database Administration** program is open.
- The external database is set up for the use in the OMNIS Software according to the instructions: *Preparing the database*

1 Starting the setup

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



A new window is opened.

2 Entering data

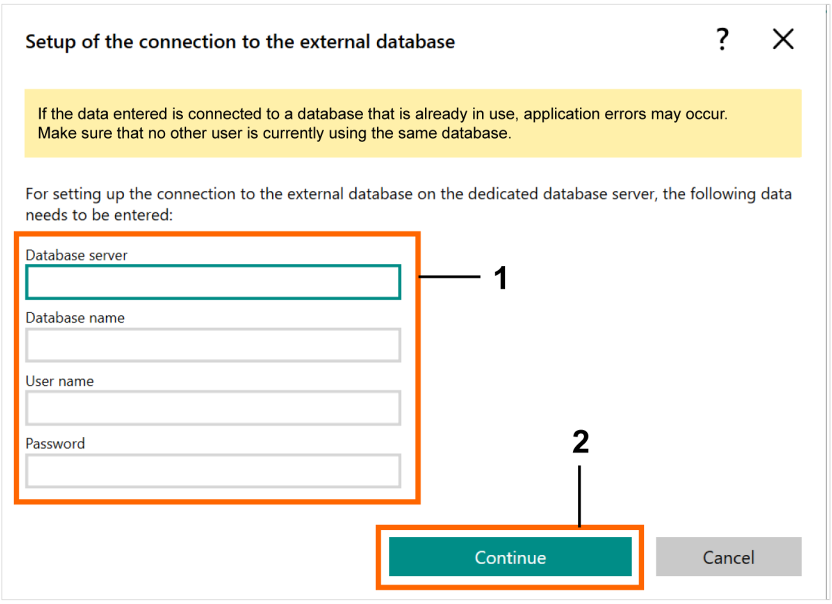
NOTICE

Application errors may occur if the data entered uses a connection to a database that is already in use. Make sure that no other user is currently using the same database.

- Enter **Database server**, **Database name**, **User name** and **Password** in the window (**1**).
- Click on **[Continue]** (**2**) to continue the setup.

NOTICE

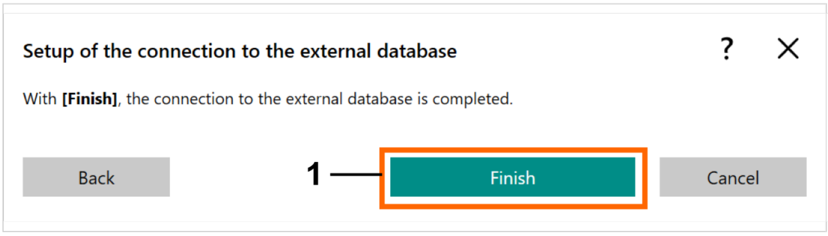
- The address of the **database server** must have the following format: **Database server address\instance, port** (e.g. 192.168.1.1\MyDatabaseServer, 1433)
  - If no default values are used for the instance and the port on the database server, **instance** and **port** must be entered as specified in the example above. The required port (default value: 1433) must be open for access.
- The **User name** must not contain any spaces.



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 ▶ Data management ▶ Connection settings**.

NOTICE

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 data must be carried out by an internal IT administrator.

NOTICE

If the connection between the OMNIS Software and the database server is interrupted, an error message appears. 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:

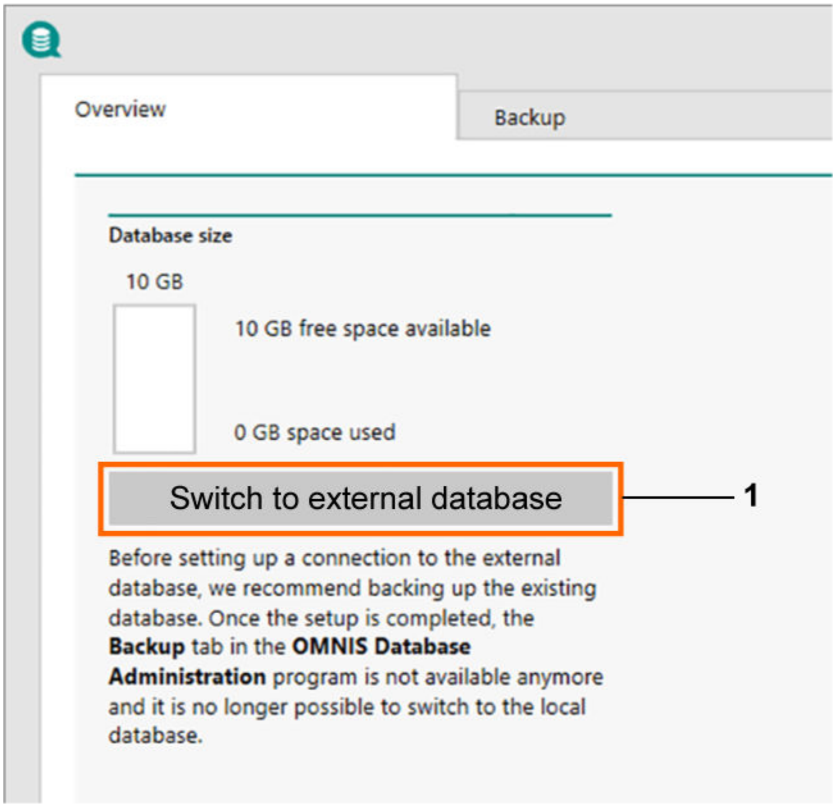
- The Windows user currently logged on has the local administrator rights.
- The **Local Microsoft SQL Server Express** option was selected on initial installation of the OMNIS Software.
- The **OMNIS Database Administration** program is open.
- The local database on the dedicated database server has been transferred according to the instructions: *Transferring the database*

1 Switching to the external database

NOTICE

Before setting up a connection to the external database, we recommend 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 data 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

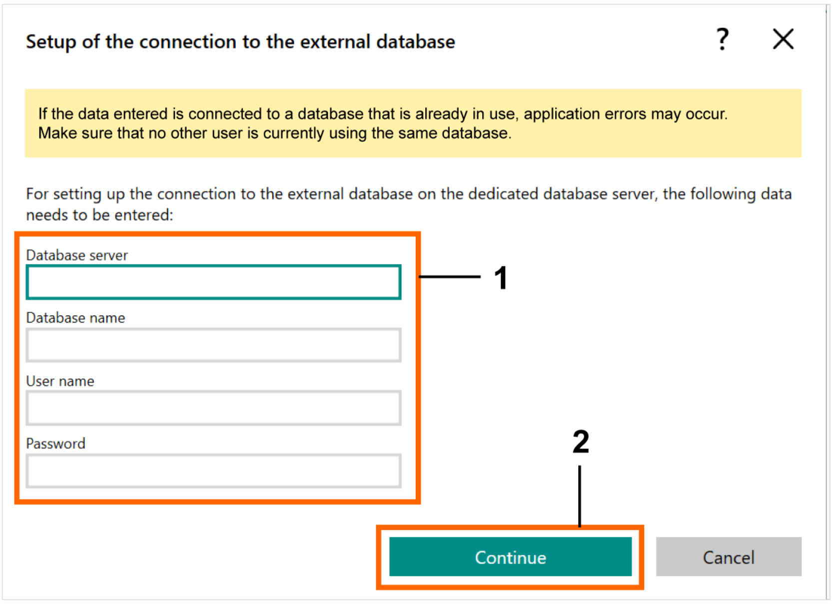
NOTICE

Application errors may occur if the data entered uses a connection to a database that is already in use. Make sure that no other user is currently using the same database.

- Enter **Database server**, **Database name**, **User name** and **Password** in the window (**1**).
- Click on **[Continue]** (**2**) to continue the setup.

NOTICE

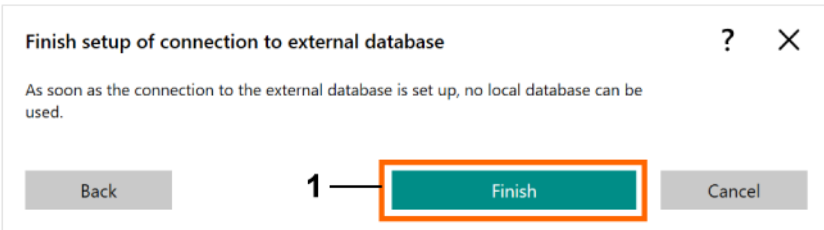
- The address of the **database server** must have the following format: **Database server address\instance, port** (e.g. 192.168.1.1\MyDatabaseServer, 1433)
  - If no default values are used for the instance and the port on the database server, **instance** and **port** must be entered as specified in the example above. The required port (default value: 1433) must be open for access.
- The **User name** must not contain any spaces.



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 ▶ Data management ▶ Connection settings**.

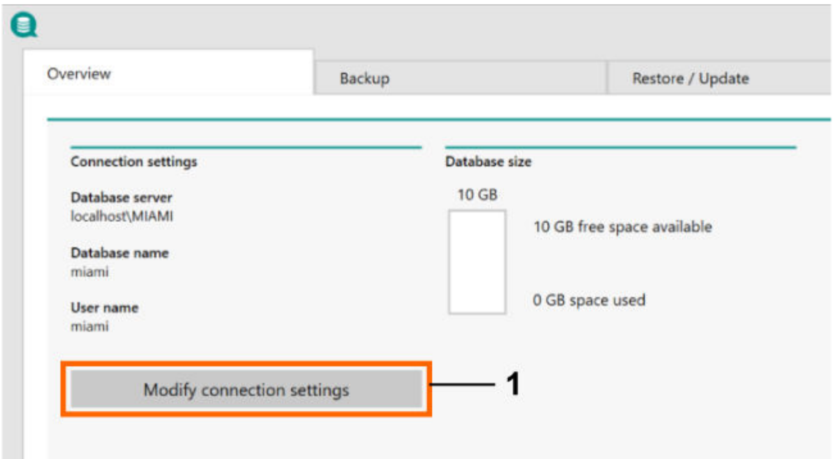
Modifying the connection settings

Prerequisite:

- The external database is installed and in use.

1 Modifying the connection settings

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



The wizard is opened where the **Database server**, **Database name**, **User name** and **Password** can be changed.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Updating the database (chapter 6.1.1, page 937)

Database – Definition (chapter 4.7, page 70)

Restoring the database (chapter 6.1.3, page 945)

Resetting the database (chapter 6.1.4, page 946)

OMNIS Database Administration – Actions (chapter 6.1, page 936)

4.8 Assigning IP addresses

Using the OMNIS 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.

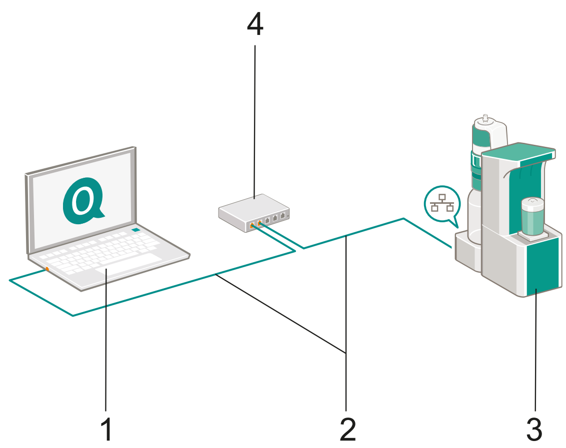
Furthermore, the user can use the OMNIS TCP/IP Service Port to define an individual host name for an OMNIS instrument.

- *(see "Typical components of a network with LAN cable connection", page 79)*
- *(see "Identifying a previously assigned IP address with connected DHCP server", page 80)*
- *(see "Resetting a previously assigned static IP address without DHCP server", page 81)*
- *(see "Changing from static IP address to dynamic IP address", page 82)*
- *(see "Assigning a static IP address", page 83)*
- *(see "Assigning a dynamic IP address", page 85)*
- *(see "Defining an individual host name", page 87)*

Typical components of a network with LAN cable connection

NOTICE

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 [icon] to open the **Inventory** window in **Equipment ▶ Instruments**.

5 **Searching for an instrument**

- Click on [icon] 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.

NOTICE

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.

NOTICE

After the reset, the OMNIS instrument still has a static IP address without DHCP server. Further information on changing to static IP address with DHCP server: *(see "Changing from static IP address to dynamic IP address", page 82)*

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 (bleep) 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* into the address line and enter the IP address noted in the last section *(see "Identifying a previously assigned IP address with connected DHCP server", page 80)* as the **IP address**. Example: *http://10.0.34.63:8080*
- Confirm the address by clicking on **[Enter]**.

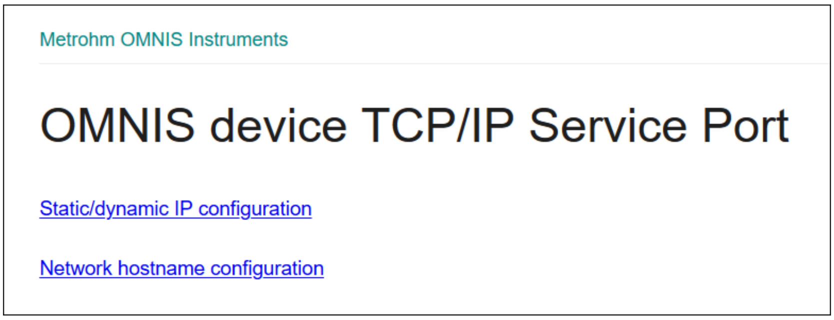
A new window is opened.

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 **Static/dynamic IP configuration** for setting an IP address.



A new window is opened.

4 Entering an IP address

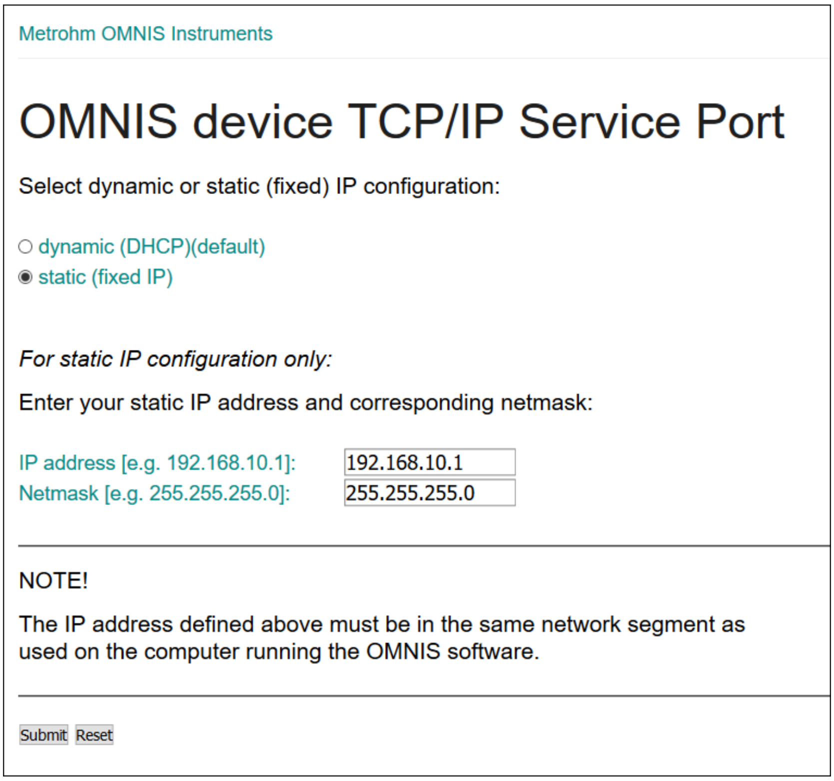
- Select the option **static (fixed IP)** for setting a fixed IP address.

- Enter the IP address noted in the last section *(see "Identifying a previously assigned IP address with connected DHCP server", page 80)* under **IP address**.
- Enter a matching netmask under **Netmask**.
- Click on **[Submit]** to confirm the entries.

NOTICE

The IP address 0.0.0.0 is invalid.

Clicking on **[Submit]** repeatedly can cause an error. If an error message is displayed, 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).

NOTICE

To find the OMNIS instrument in the network, the IP address defined above must be on the same network as the computer on which the OMNIS Software is being run.

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* into the address line and enter the IP address noted in the last section *(see "Identifying a previously assigned IP address with connected DHCP server", page 80)* as the **IP address**. Example: *http://10.0.34.63:8080*.
- Confirm the address by clicking on **[Enter]**.

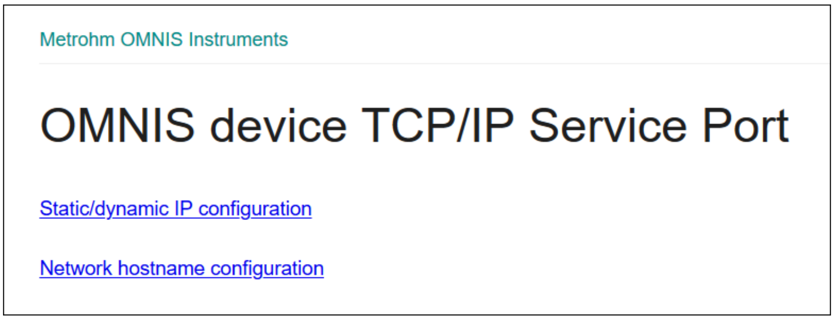
A new window is opened.

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 **Static/dynamic IP configuration** for setting an IP address.



A new window is opened.

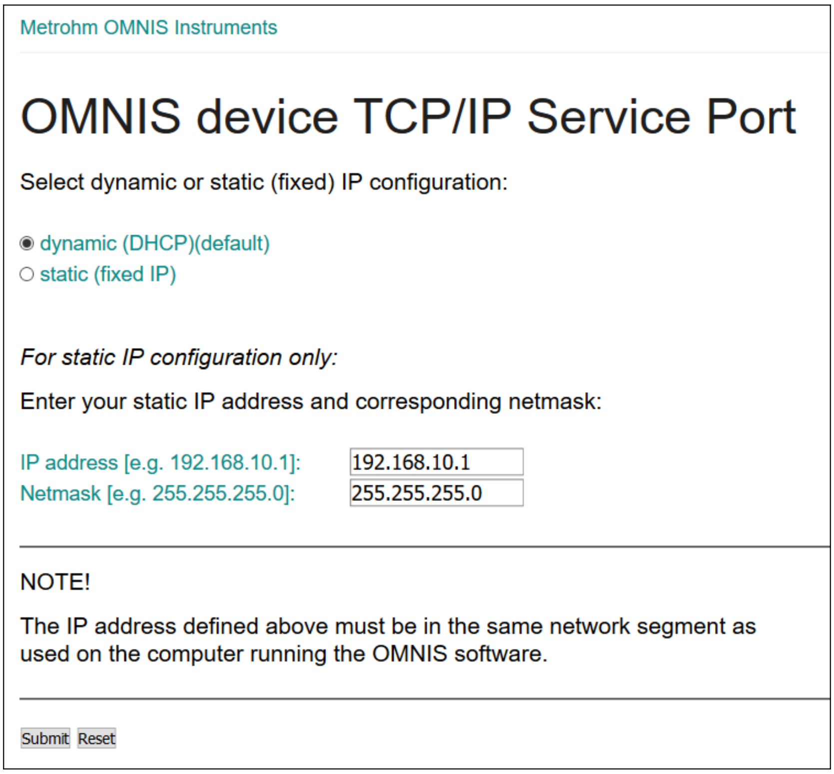
4 Entering an IP address

- Select the option **dynamic (DHCP) (default)** for setting a dynamic IP address.
- Enter the IP address noted in the last section *(see "Identifying a previously assigned IP address with connected DHCP server", page 80)* under **IP address**.
- Enter a matching netmask under **Netmask**.
- Click on **[Submit]** to confirm the entries.

NOTICE

The IP address 0.0.0.0 is invalid.

Clicking on **[Submit]** repeatedly can cause an error. If an error message is displayed, 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).

NOTICE

To find the OMNIS instrument in the network, the IP address defined by the DHCP server must be on the same network as the computer on which the OMNIS Software is being run.

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]**.

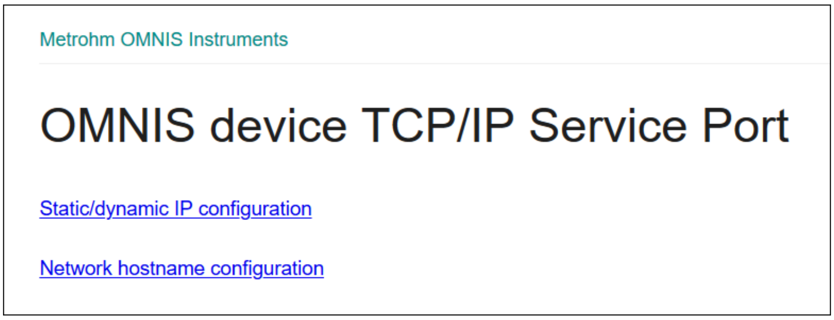
A new window is opened.

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 **Network hostname configuration** option for configuring the product name in the network.



A new window is opened.

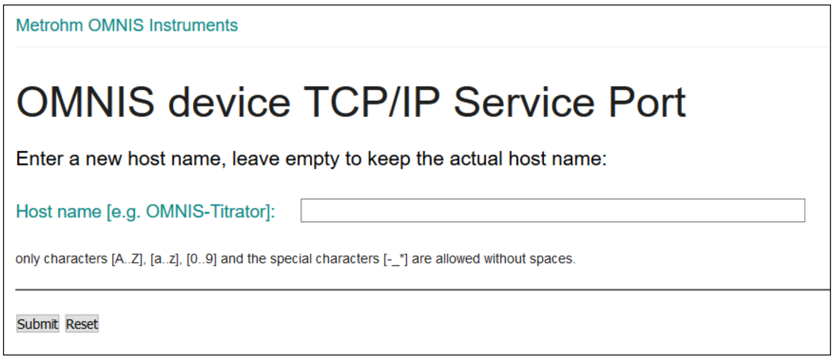
4 Entering a host name

- Enter the host name of the OMNIS instrument in the **Host name** input field.
- Click on **[Submit]** to confirm the entries.

NOTICE

The host name must contain at least 3 characters.

Clicking on **[Submit]** repeatedly can cause an error. If an error message is displayed, 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).

NOTICE

The host name of the OMNIS instrument is reset once again after a firmware update on an OMNIS instrument.

See also

Reserving instruments (chapter 5.10.1.3, page 666)

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.

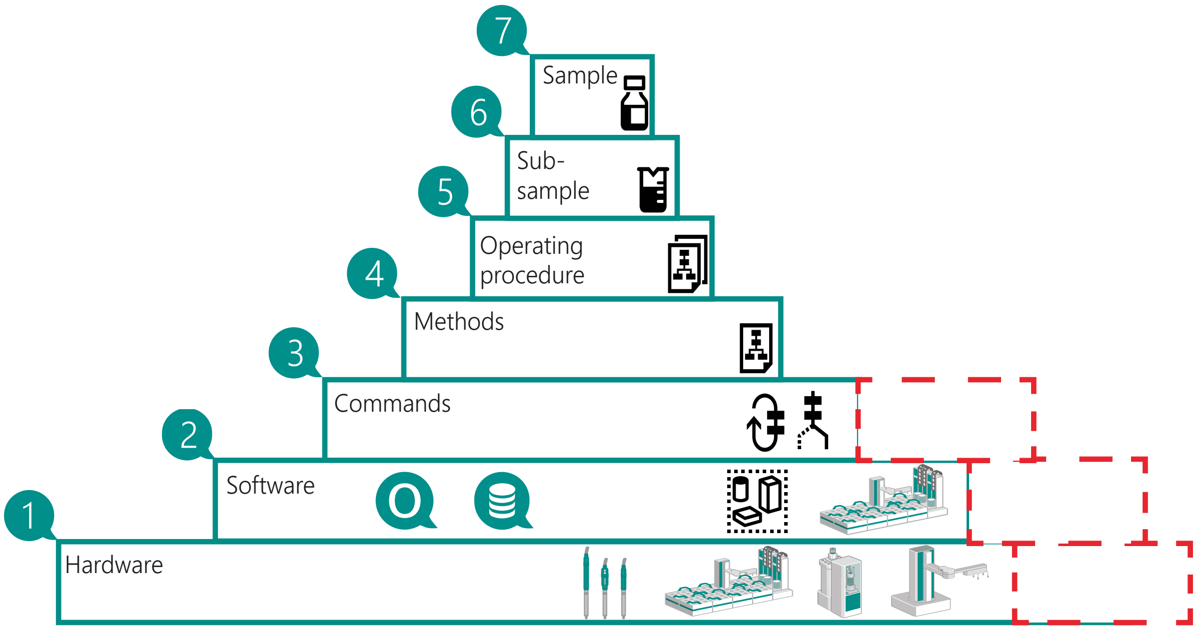


Figure 2 Overview of the OMNIS system from the hardware to the sample.

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.

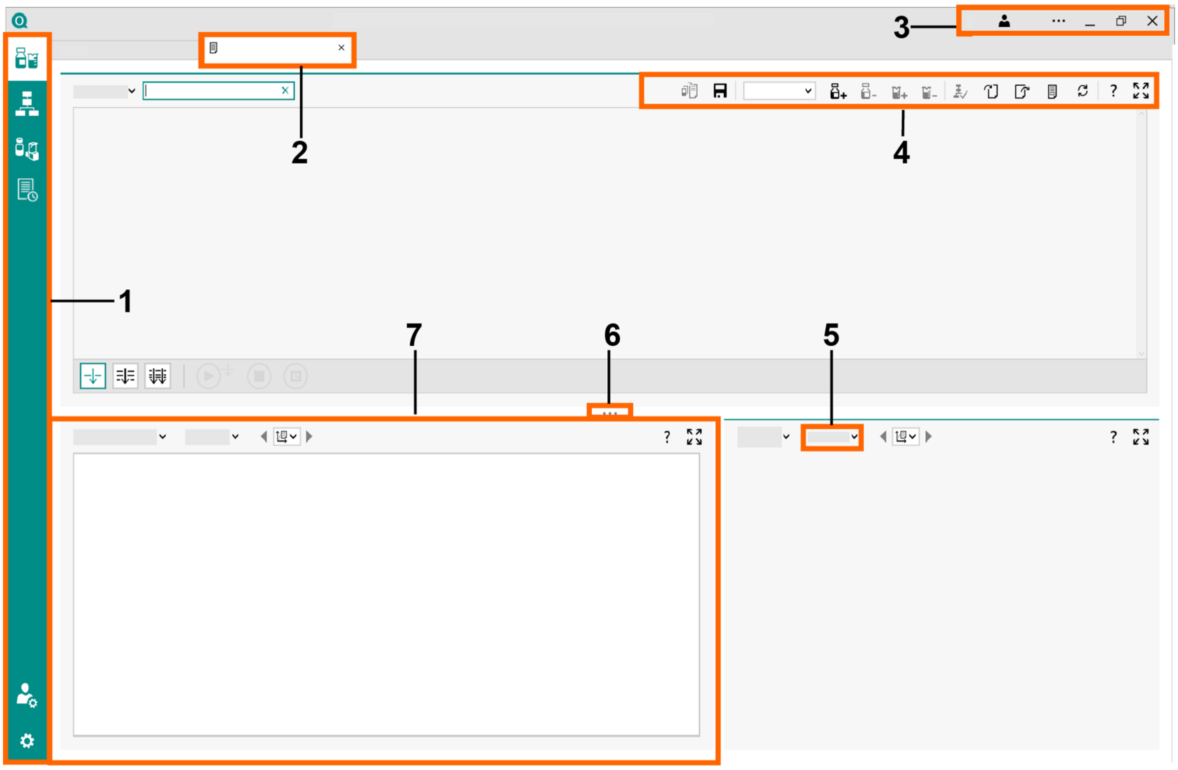
6 Subsamples
Subsamples are part of a sample. A different determination can be carried out for each subsample. An operating procedure must be assigned to each subsample for this reason.

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

Overview of the user interface

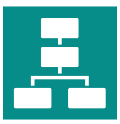


1	**Work areas**	**2**	**Tab**
3	**Icons in the title bar (for the entire OMNIS Software)**	**4**	**Icons for that area**
5	**Subsection**	**6**	**Separating bar**
7	**Area**		

Work area

The following work areas are displayed on the navigation bar (**1**):

Samples



Processes

Equipment

Audit trail

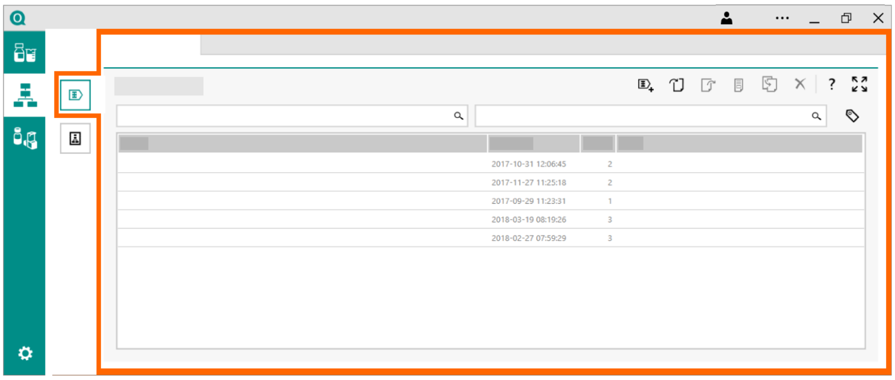
User management

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.

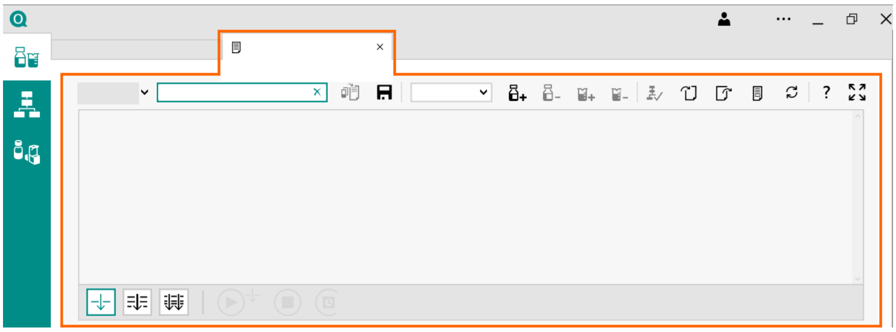
Example: The **Operating procedures** subsection in the **Processes** work area



Tab

A tab (**2**) is created as soon as a new object (e.g. operating procedure, sample list, etc.) is created. The user can switch between multiple opened tabs. Tabs can also be closed again individually.

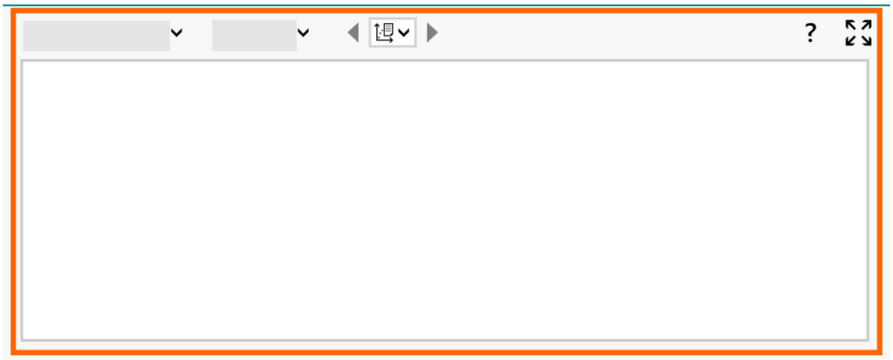
Example: The **New sample list** tab in the **Samples** work area



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

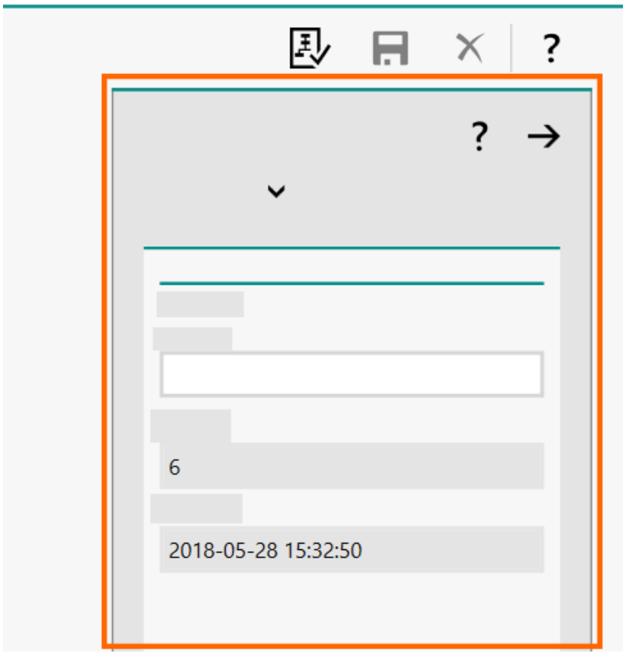


The size of the individual areas can be adapted using the horizontal and vertical separating bar (**6**) by pulling the areas in the desired direction while holding the mouse button pressed down.

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.

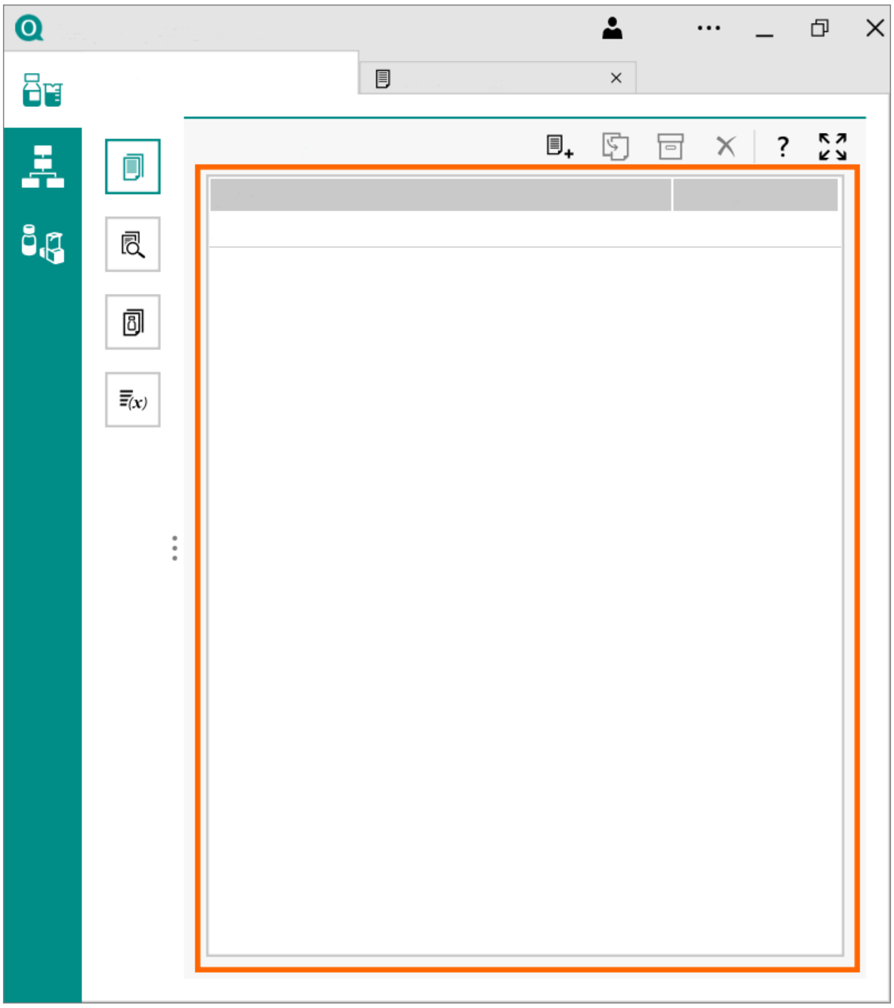
Example: The **Properties** window in the **New method** tab



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:



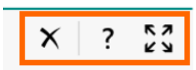
In each table, the entries of a column can be sorted by clicking with the left mouse button on the desired column head. A triangle on the left in the column head indicates the column according to which the current sorting has been performed and whether the entries are sorted in ascending or descending order.

Icons

Icons with which certain functions can be initiated or further areas can be opened are available not only for the title bar (**6**) but also for the individual areas (**7**).

Example (6):

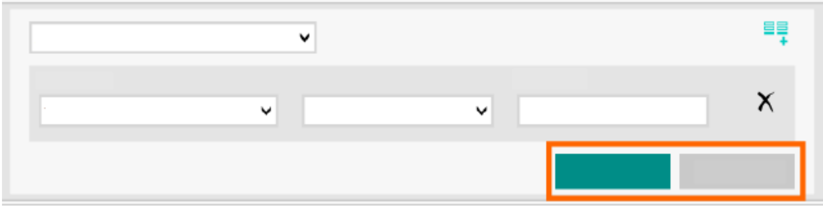
Example (7):



Buttons

Buttons are used to initiate actions and, unlike icons, they feature textual information on their functionality. (e.g. **[Filter]**).

Example:



See also

User rights – Directory (chapter 4.6.7.3, page 62)

OMNIS Software – System overview (chapter 5.1, page 90)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Samples – Definition (chapter 5.8.3, page 171)

Processes – Actions (chapter 5.9, page 259)

Equipment – Actions (chapter 5.10, page 659)

Audit trail work area – Actions (chapter 5.12, page 917)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

Setting up OMNIS Software (chapter 4.3, page 17)

5.2.1 Library – Brief description

Clicking on in **Processes ▶ Operating procedures** or **Processes ▶ Methods** opens the **Library** window. The following subsections can be selected here:

For operating procedures

- **Methods**
  Here you will find all methods saved.
- **Commands**
  Here you will find all commands which can be inserted into an operating procedure.
- **Optional runs**
  Here you will find the optional runs which can be inserted into an operating procedure.

For methods

- **Commands**
  Here you will find all commands which can be inserted in a method.
- **Optional runs**
  Here you will find the optional runs which can be inserted in a method.

NOTICE

Brief descriptions of the functions of the commands or the optional runs can be found in the tooltips and more detailed information in the OMNIS Help

NOTICE

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.

See also

Operating procedure – Definition (chapter 5.9.1, page 260)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Method – Definition (chapter 5.9.2, page 281)

Creating and editing a method (chapter 5.9.2.3, page 284)

Commands – Definition (chapter 5.9.4, page 293)

Run in case of an error – Definition (chapter 5.9.3.1, page 291)

Run in case of a stop – Definition (chapter 5.9.3.2, page 292)

Run in case of a limit value violation – Definition (chapter 5.9.3.3, page 293)

5.2.2 OMNIS Software – Inventory

This topic describes the **Inventory** window in the subsections **Instruments**, **Sensors** and **Solutions** of the work area **Equipment**, and on the tab **Work system**.

Clicking on opens the **Inventory** window. All of the instruments, functional units, sensors and solutions available in the network are displayed in this. Drag and drop can be used to reserve these instruments or to add sensors and solutions to the sensor list or the solution list.

All of the functional units available on the reserved instruments are displayed on the **Work system** tab. These functional units can be added to the work system via drag and drop.

NOTICE

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, it can be entered in the search field. Then only the instruments which fulfil the entered search criteria are listed.

See also

Reserving instruments (chapter 5.10.1.3, page 666)

Creating a work system (chapter 5.10.3.2, page 785)

Instruments – Directory (chapter 5.10.1.1, page 660)

Functional unit – Directory (chapter 5.10.2.1, page 697)

Solution – Definition (chapter 5.10.6, page 818)

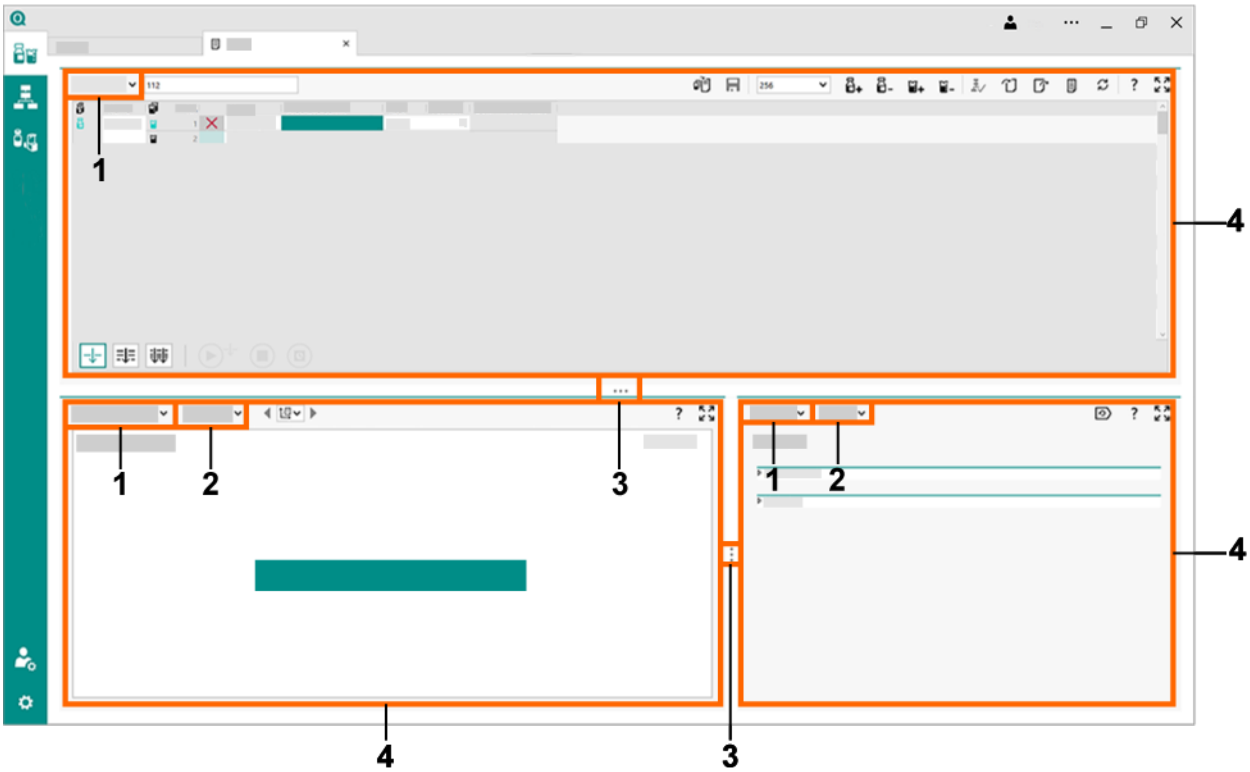
Sensor – Definition (chapter 5.10.5, page 794)

Sensor – Properties (chapter 5.10.5.2, page 798)

pH electrode – Calibrating (chapter 5.10.5.4, page 803)

Ion-selective electrode – Calibrating (chapter 5.10.5.5, page 805)

5.2.3 Sample list – Tab



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	**Separating bar** The size of the individual areas can be adjusted with the separating bar.	**4**	**Area** Display the selected area.

Sample list

1 Managing determinations

Define the determination type (single determination, series determination, parallel determination). Start, stop or pause a determination.

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 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.

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**	**Icons** Further information on the functions of the individual icons: *OMNIS Software – Overview of functions (see chapter 5.3, page 119)*
9	**Selecting a sample profile** A sample profile can be selected from the selection list.	**10**	**Selecting the operating procedure** An operating procedure can be selected for the subsample from the selection list.

Results

- **Raw data**
  Raw data of a result (e.g. of an equivalence point) as well as determination data are displayed here.
- **Predictions**
  Here, calculations for spectra 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.

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** and **History** 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 subsample, subsample determination and history overview are recorded and displayed chronologically here.
- **Signatures**
  Signatures of subsamples are displayed here.

NOTICE

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

Operating procedures – Subsection (chapter 5.9.1.1, page 261)

Restoring operating procedure and associated methods (chapter 5.9.1.7, page 273)

Methods – Subsection (chapter 5.9.2.1, page 282)

Predictions – Subsection (chapter 5.8.23, page 255)

Reevaluating the prediction (chapter 5.8.23.1, page 256)

Report template – Directory (chapter 5.8.1.4, page 155)

Displaying the results (chapter 5.8.18, page 241)

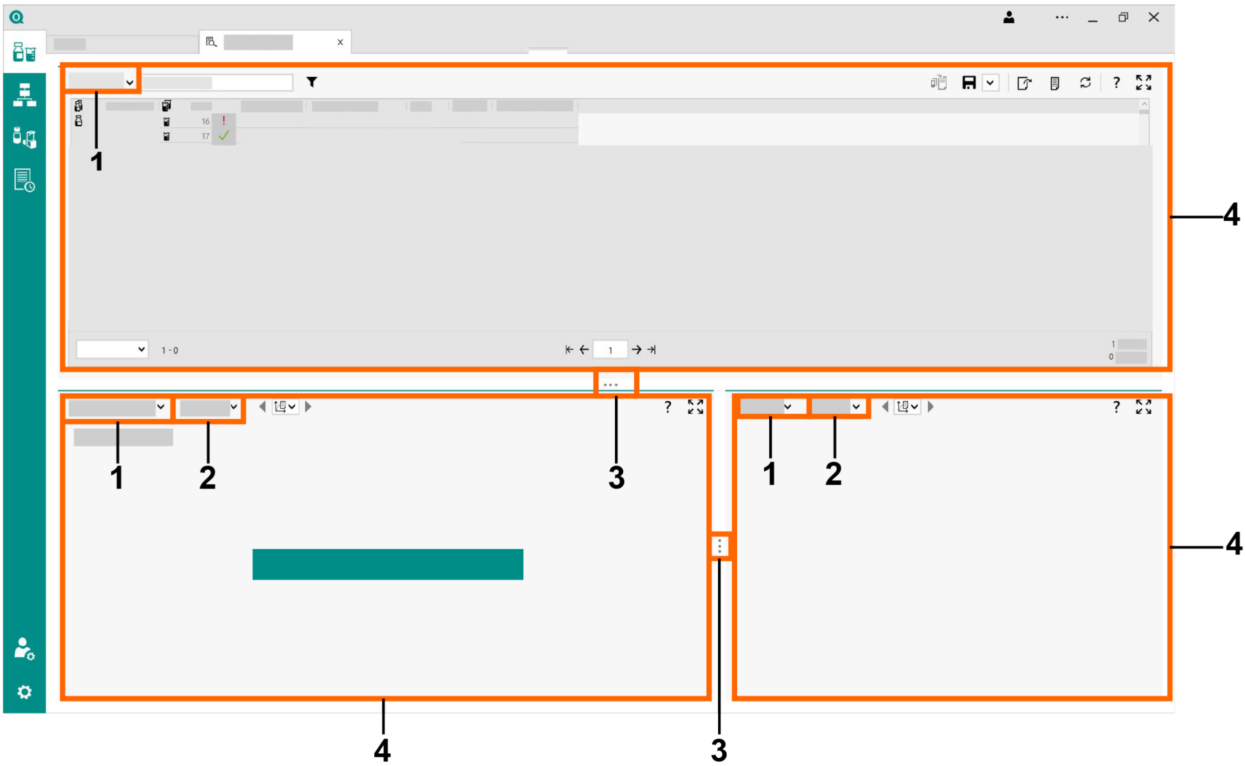
Sample lists – Subsection (chapter 5.8.1, page 141)

Signature – Brief description (chapter 5.6, page 131)

Displaying a signature (chapter 5.6.2, page 134)

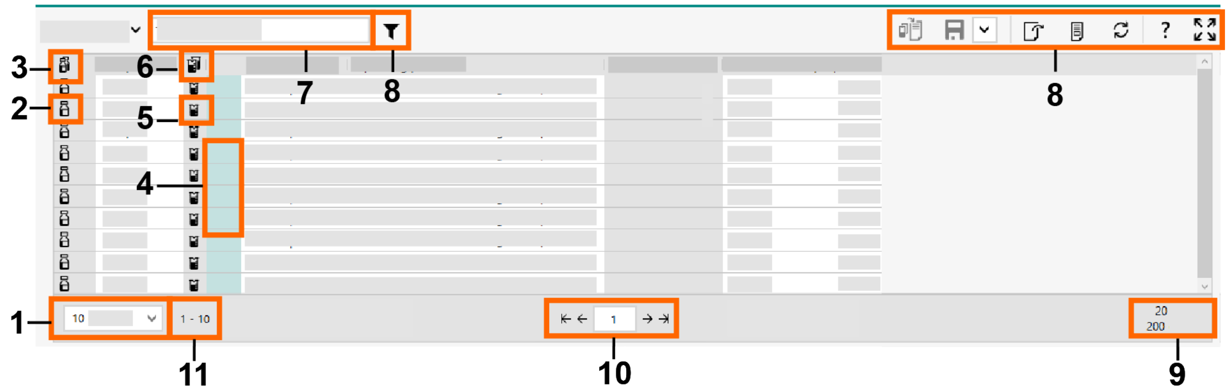
Monitoring – Definition (chapter 5.8.22, page 251)

5.2.4 Search query – Tab



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	**Separating bar** The size of the individual areas can be adjusted with the separating bar.	**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 / 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 / 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 Icons

Further information on the functions of the individual icons: *OMNIS Software – Overview of functions (see chapter 5.3, page 119)*

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

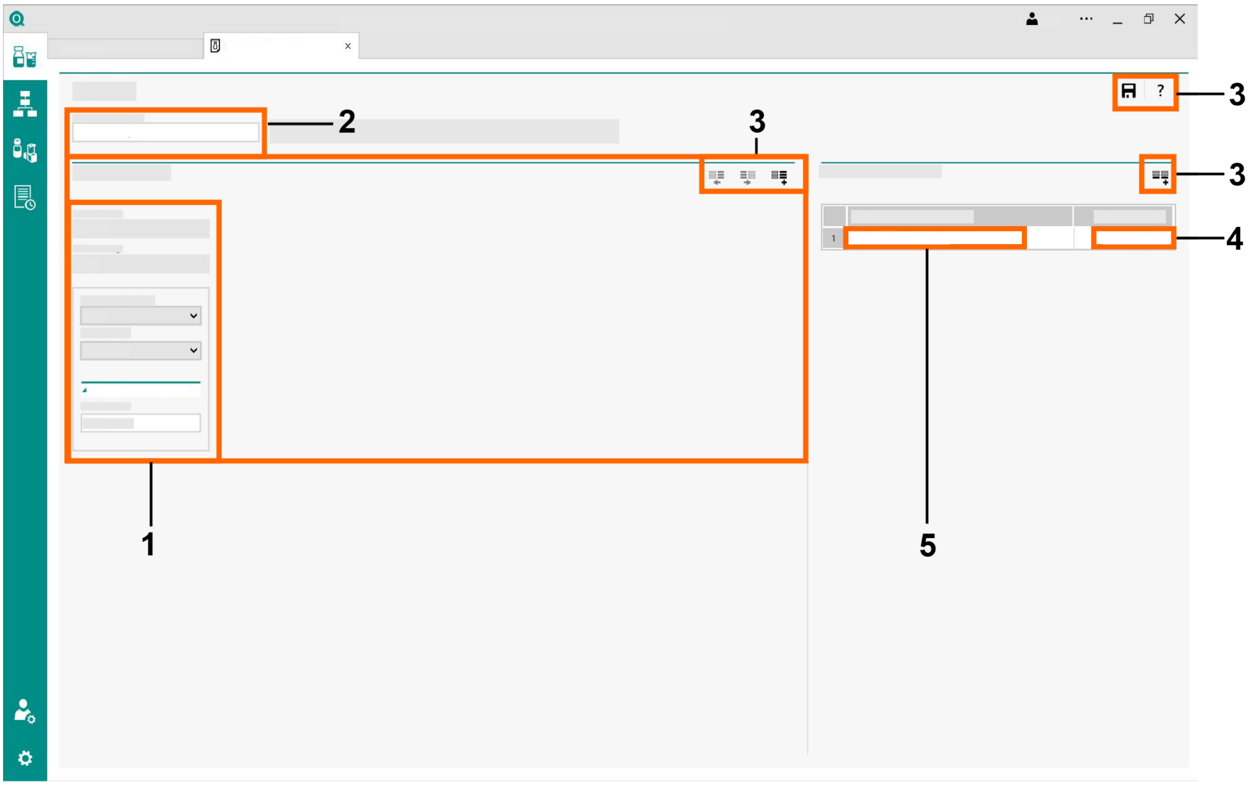
Sample list – Tab (chapter 5.2.3, page 100)

Creating a Search queries (chapter 5.8.2.2, page 166)

Filtering Search queries (chapter 5.8.2.3, page 167)

Subsamples – Definition (chapter 5.8.5, page 180)

5.2.5 Sample profile – Tab



1	**Sample data** Define sample data that is available as sample identification.	**2**	**Name field** The name of the sample profile can be changed here.
3	**Icons** Further information on the functions of the individual icons: *OMNIS Software – Overview of functions (see chapter 5.3, page 119)*	**4**	**Entering a 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

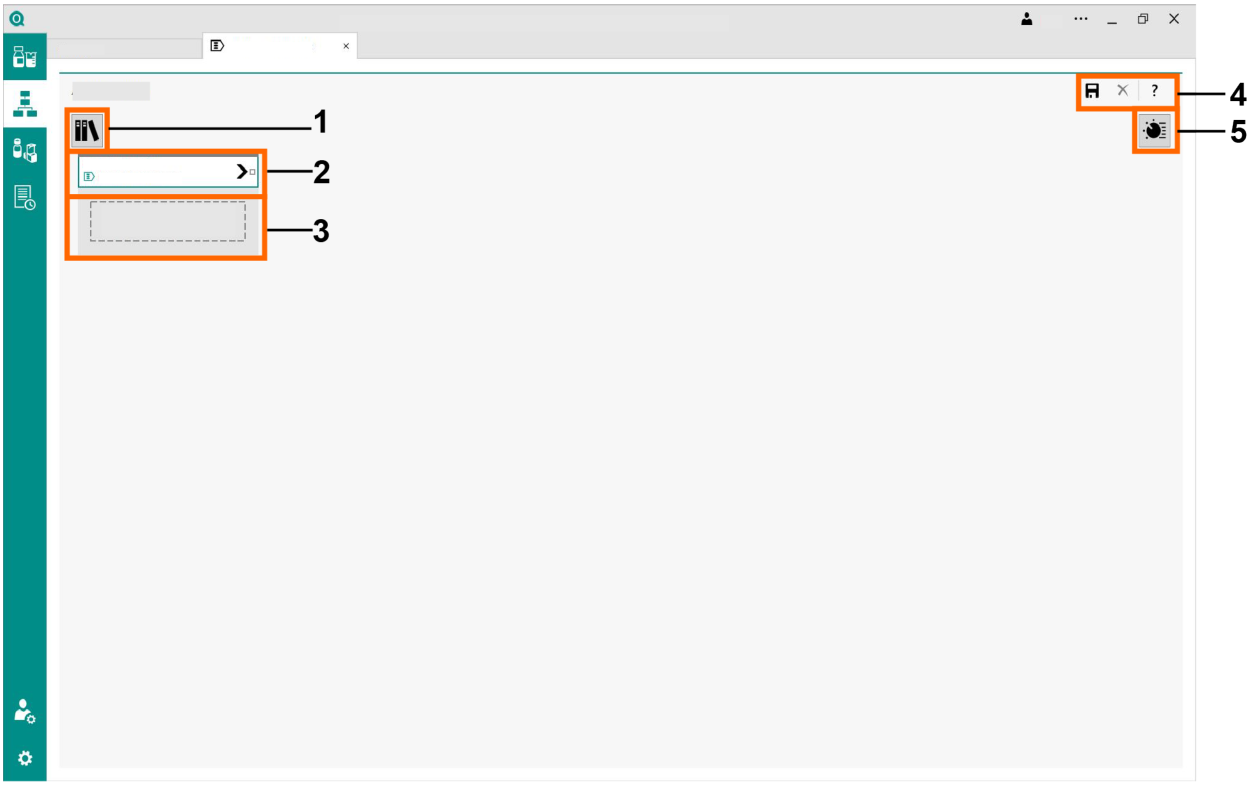
Operating procedure – Definition (chapter 5.9.1, page 260)

Sample profile – Definition (chapter 5.8.4, page 176)

Creating and editing a sample profile (chapter 5.8.4.1, page 176)

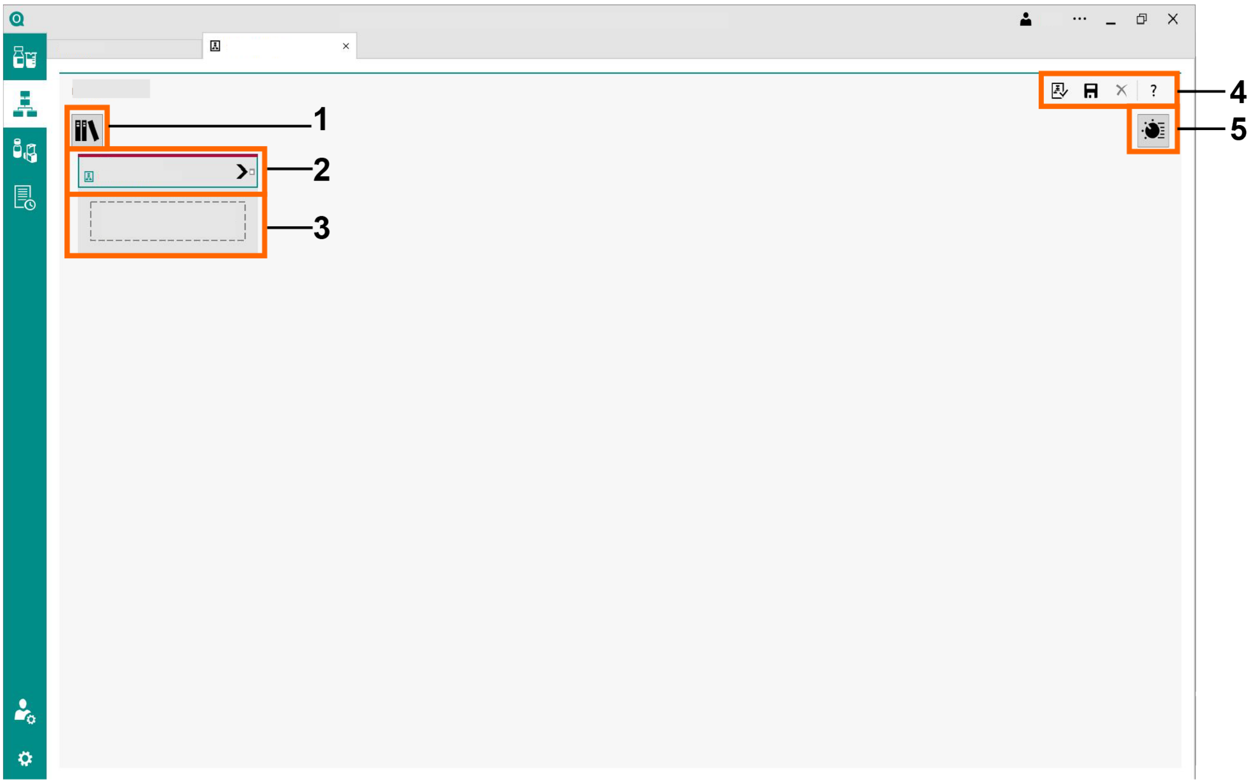
5.2.6 Operating procedure and method – Tab

Operating procedure



1	**Library** Open a list with all available commands, methods and optional runs.	**2**	**Defining a new operating procedure** Double-click on the icon of the operating procedure to open the **Properties** window directly in order to view or edit the properties of the selected element.
3	**Compiling a new operating procedure** Use drag and drop to insert the desired elements from the library into the operating procedure.	**4**	**Icons** Further information on the functions of the individual icons: *OMNIS Software – Overview of functions (see chapter 5.3, page 119)*
5	**Properties** Different functions and information are available from the subsections **General**, **Parameters**, **Execute with**, **Result monitoring**, **Reports** and **Export**, depending on the element selected.		

Method



1 Library
Open a list with all available commands and optional runs.

2 Defining a new method
Double-click on the icon of the method to open the **Properties** window directly in order to view or edit the properties of the selected element.

3 Compiling a new method
Use drag and drop to insert the desired elements from the library into the method.

4 Icons
Further information on the functions of the individual icons: *OMNIS Software – Overview of functions (see chapter 5.3, page 119)*

5 Properties
Different functions and information are available from the subsections **General**, **Parameters** and **Execute with**, depending on the element selected.

See also

Operating procedure – Definition (chapter 5.9.1, page 260)

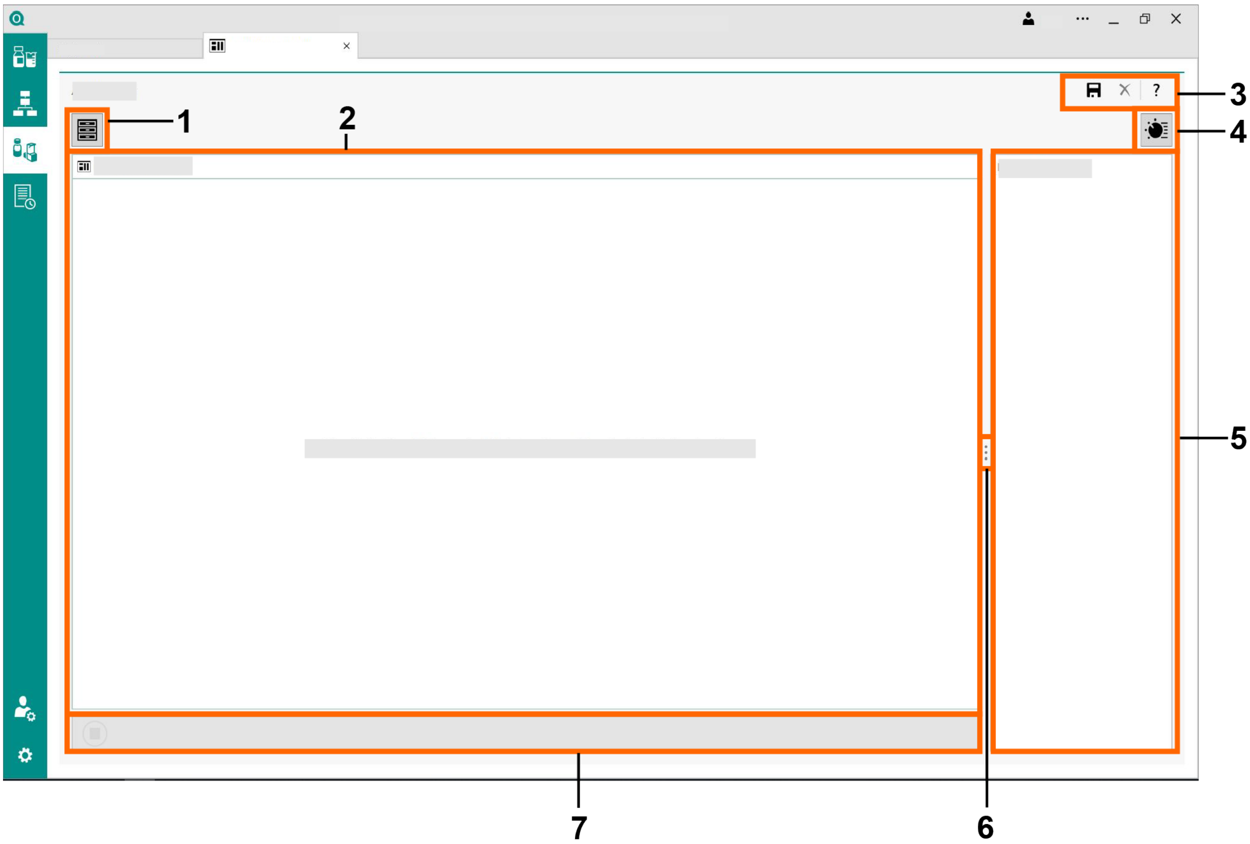
Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Operating procedures – Subsection (chapter 5.9.1.1, page 261)

Method – Definition (chapter 5.9.2, page 281)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.2.7 Work system – Tab



1 Inventory Open a list with all available functional units.	**2 Compiling a new work system** Use drag and drop to insert the desired functional units from the inventory into the work system.
3 Icons Further information on the functions of the individual icons: *OMNIS Software – Overview of functions (see chapter 5.3, page 119)*	**4 Properties** Different functions and information are available in the subsection **General**, depending on the element selected.

5 Running processes

Running processes are 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 Separating bar

The size of the individual areas can be adjusted with the separating bar.

7 Stopping 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, it cannot be stopped.

See also

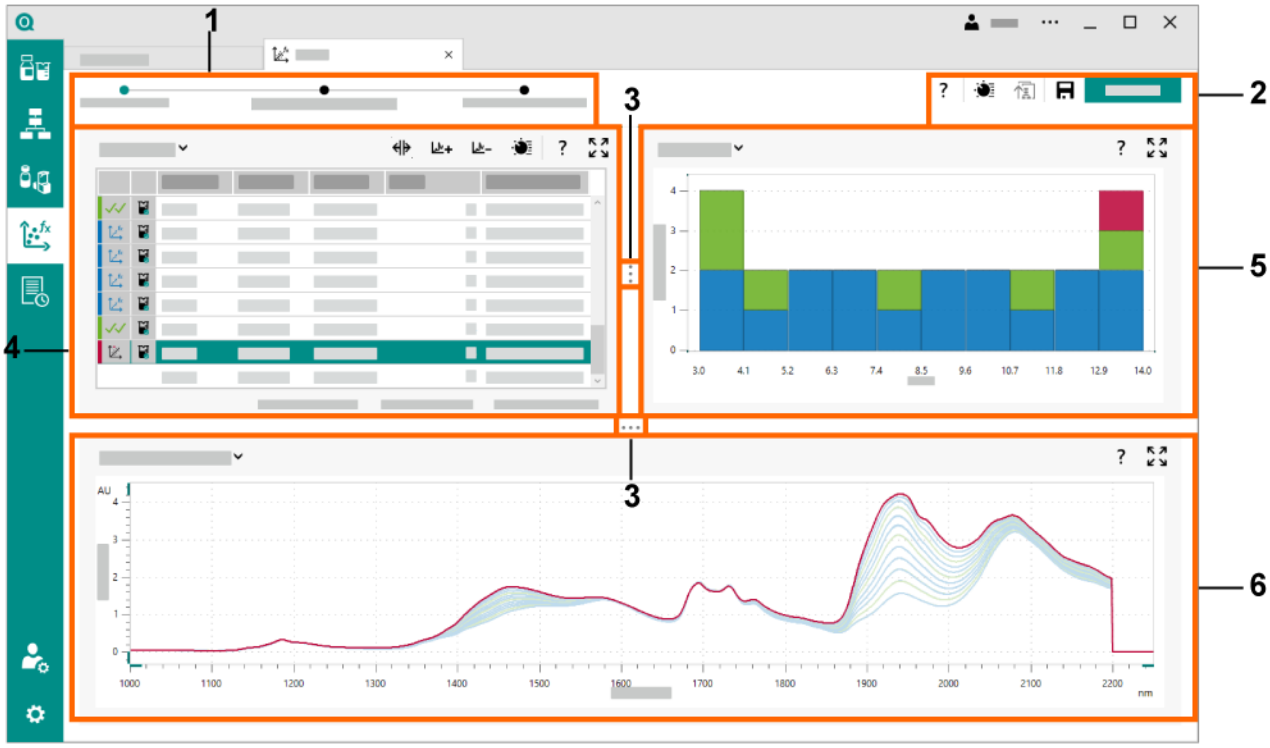
Work system – Definition (chapter 5.10.3, page 783)

Creating a work system (chapter 5.10.3.2, page 785)

Functional unit – Definition (chapter 5.10.2, page 696)

5.2.8 Prediction model – Tab

"Select samples" process step



1 **Prediction model navigator**
Selection from process steps **Select samples**, **Parameterize prediction model** and **Validate prediction model**. *Prediction model navigator – Functional description (see chapter 5.11.1.6, page 883)*

2 **Calculation and icons**
Calculate, save and publish the prediction model.

Further information on the functions of the individual icons: *OMNIS Software – Overview of functions (see chapter 5.3, page 119)*

3 **Separating bar**
The size of the individual areas can be adjusted with the separating bar.

4 **Spectra list**
The spectra that are used in the prediction model are displayed here. See detailed image *Spectra list*.

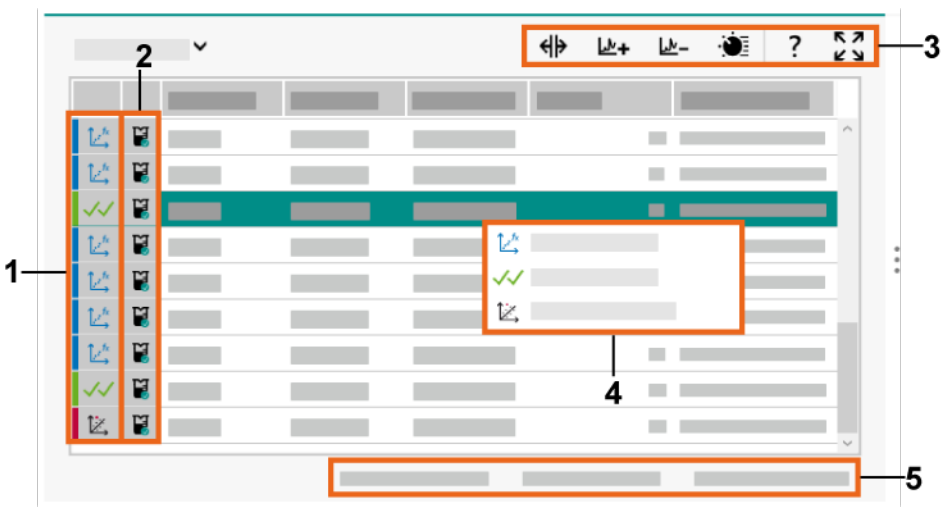
Selecting a spectrum in the list also causes that spectrum to be highlighted in the spectra overlay, in the correlation plot and in the influence plot.

5 **Histogram**
The frequency distribution of data sets of the reference parameter is displayed here. *Histogram – Area (see chapter 5.11.1.9, page 889)*

6 **Spectra overlay**
Here the untreated spectra from the spectra list are displayed overlaid. *Spectra overlay – Area (see chapter 5.11.1.10, page 890)*

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 **Data set display**
Shows the data set to which the spectrum belongs.

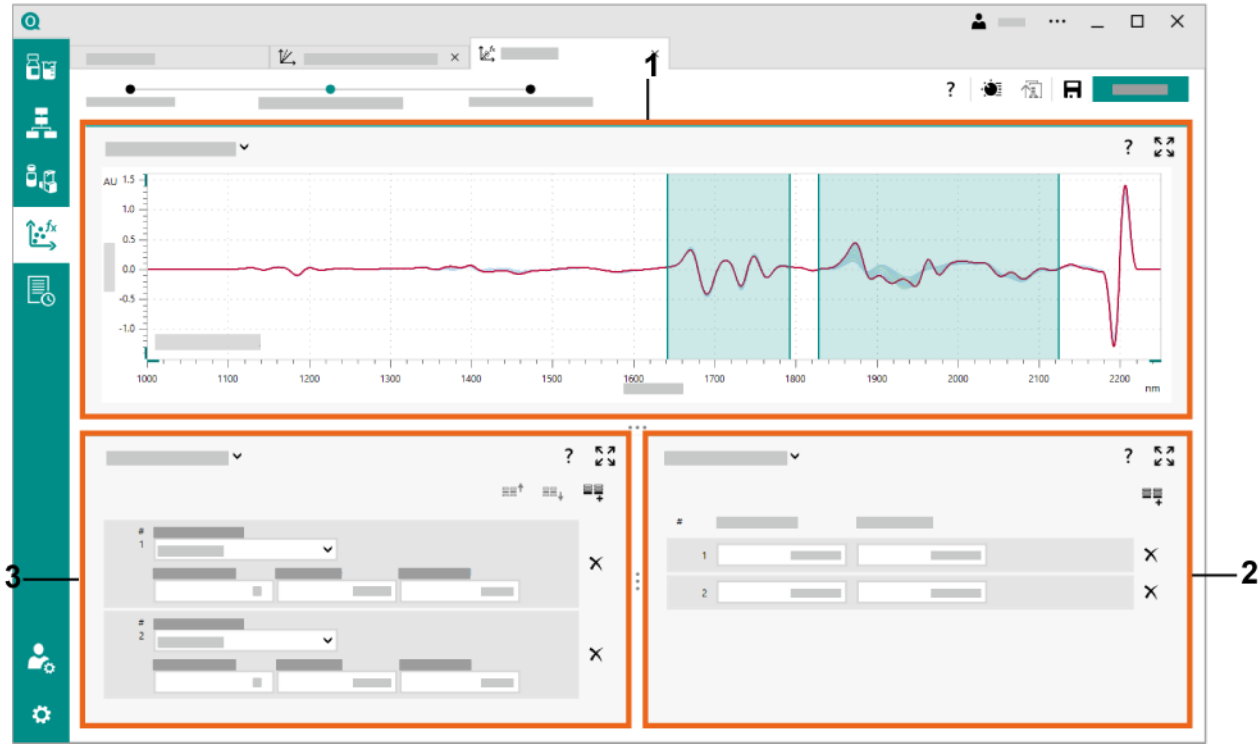
2 **Availability of the subsample in the database**
Shows whether the subsample is available in the database.

3 **Icons**
Further information on the functions of the individual icons: *OMNIS Software – Overview of functions (see chapter 5.3, page 119)*

4 **Context menu**
With the context menu, a spectrum can be assigned to a data set.

5 **Number of spectra per data set**
Shows the number of spectra in the individual data sets.

"Parameterize prediction model" process step

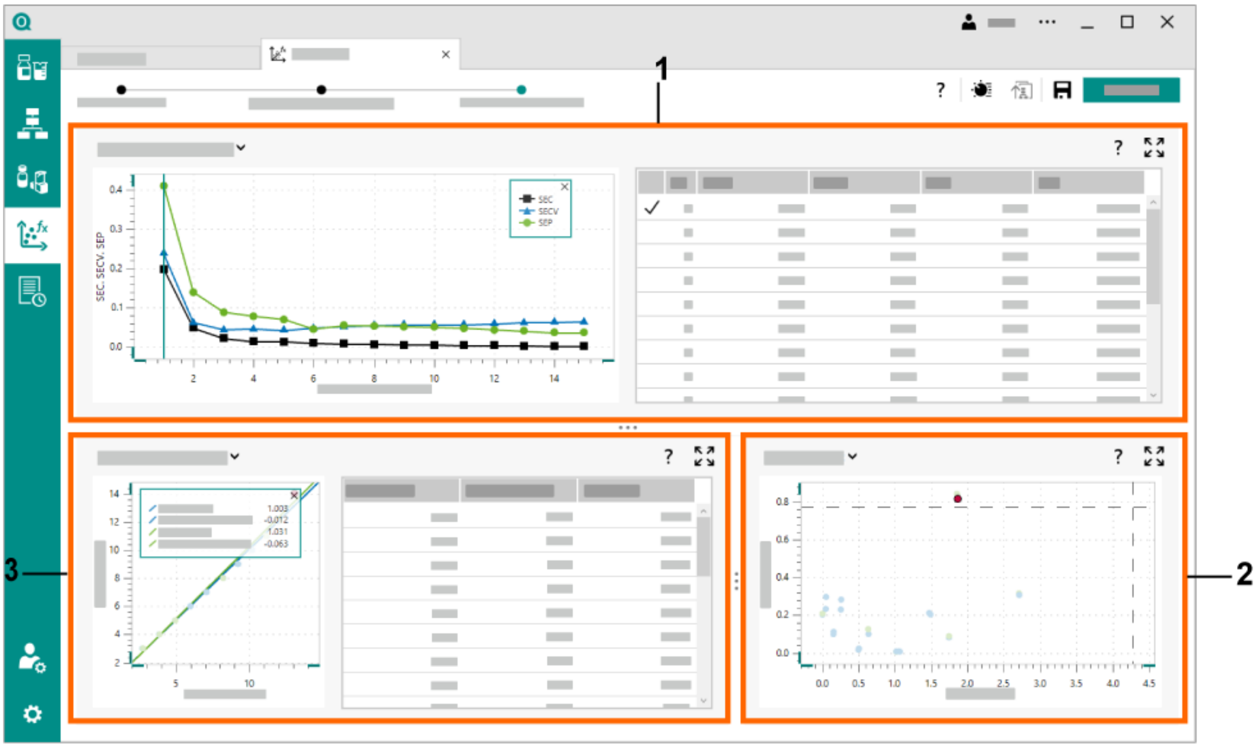


1 Spectra overlay
Here the preprocessed spectra from the spectra list are displayed overlaid. *Spectra overlay – Area (see chapter 5.11.1.10, page 890)*

3 Data preprocessing
Here the desired procedures for the data preprocessing of spectra are selected and the order in which they are applied is determined. *Data preprocessing – Area (see chapter 5.11.1.11, page 890)*

2 Wavelength range
Here you can select the desired wavelength range of the spectra overlay that is used for the calculation of the prediction model. *Wavelength range – Area (see chapter 5.11.1.12, page 892)*

"Validate prediction model" process step



1 Figures of merit
The figures of merit for a number of latent variables are displayed here. The values are displayed as a chart and as a table. *Figures of merit – Definition (see chapter 5.11.1.14, page 896)*

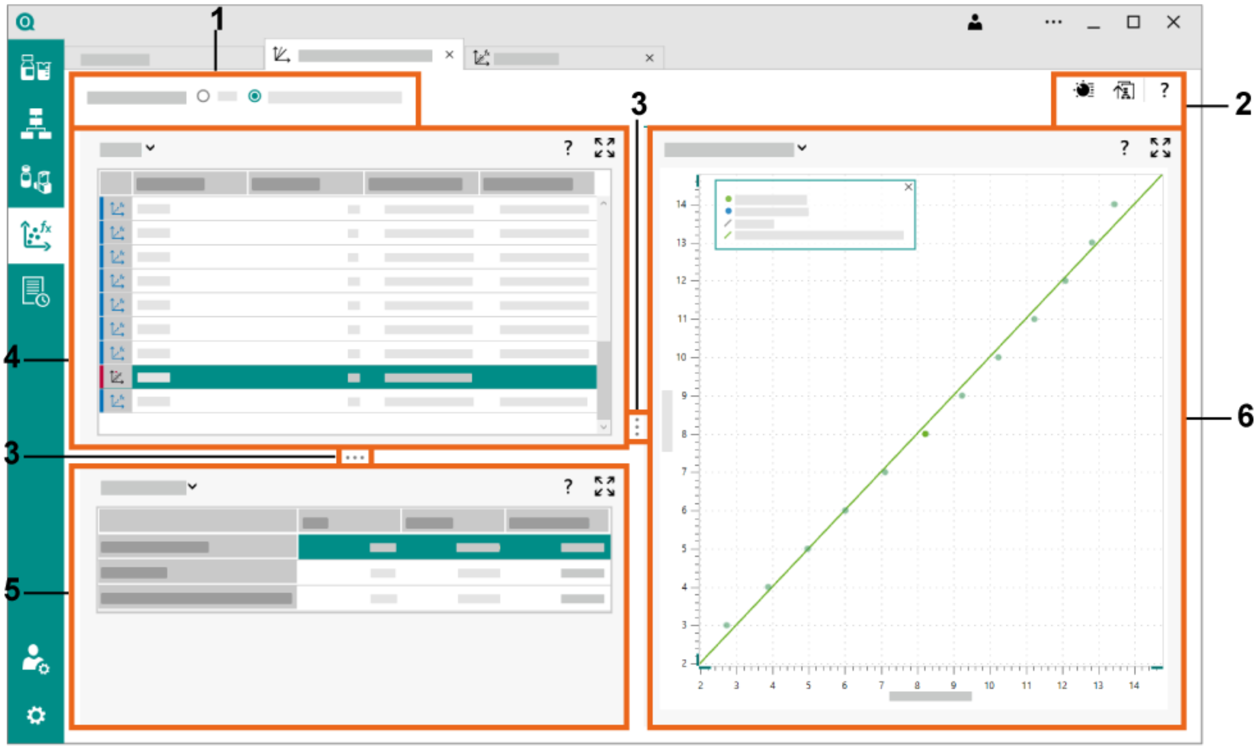
2 Influence plot
Here, the identification of outliers is made possible. *Influence plot – Area (see chapter 5.11.1.16, page 902)*

3 Correlation plot
The correlation of the measured quantities **Reference value** and **Calculated value** are displayed here. The values are displayed as a chart and as a table. The assignment to the calibration data set or validation data set is shown in color.*Correlation plot – Area (see chapter 5.11.1.15, page 898)*

See also

Prediction model – Definition (chapter 5.11.1.1, page 866)

5.2.9 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: *Slope/y-intercept correction – Definition (see chapter 5.11.2.7, page 915)*

2 Icons
Further information on the functions of the individual icons: *OMNIS Software – Overview of functions (see chapter 5.3, page 119)*

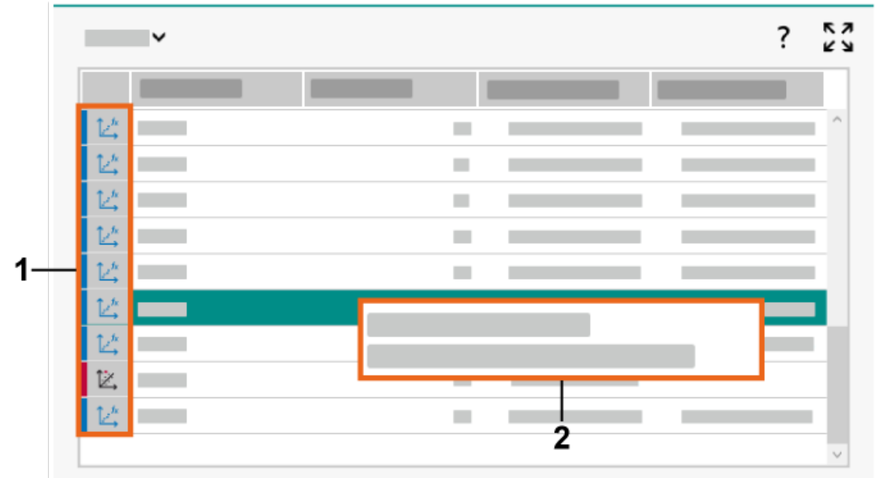
3 Separating bar
The size of the individual areas can be adjusted with the separating bar.

4 Samples
The samples whose data are used for the calculation of the slope/y-intercept correction are displayed here. See detailed image *Samples*.

5 Correction values
Here the values **SEP**, **Slope** and **y-intercept** (calculated y-intercept coefficient) are displayed respectively without correction, with bias correction and with slope/y-intercept correction. *Calculations – Definition (see chapter 5.8.19, page 243)*

6 Correlation plot
The correlation of the constituent value and the predicted or corrected value are displayed here. Further information on the correlation plot: *Correlation plot – Area (see chapter 5.11.1.15, page 898)*

Samples



1 **Data set display**
Shows whether the spectrum is included in the calculation or whether it is marked as an outlier.

2 **Context menu**
The context menu can be used to mark a spectrum as an outlier.

See also

Slope/y-intercept correction – Definition (chapter 5.11.2.7, page 915)

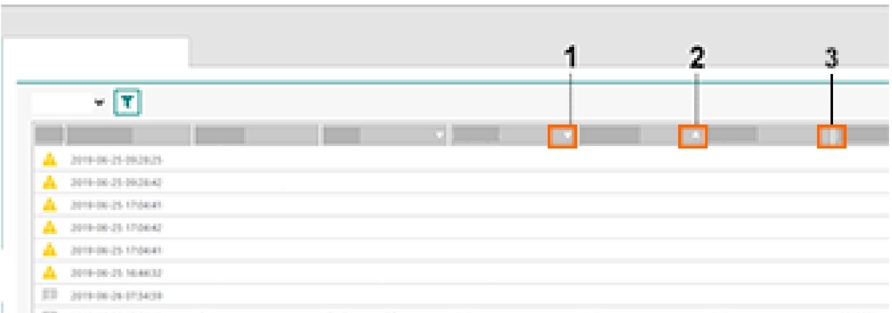
Prediction model – Definition (chapter 5.11.1.1, page 866)

Correlation plot – Area (chapter 5.11.1.15, page 898)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

5.2.10 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**).

NOTICE

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

User interface OMNIS Software – Overview (chapter 5.2, page 92)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

User rights – Directory (chapter 4.6.7.3, page 62)

Samples – Actions (chapter 5.8, page 140)

Processes – Actions (chapter 5.9, page 259)

Audit trail work area – Actions (chapter 5.12, page 917)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (OMNIS) – Actions (chapter 4.6, page 23)

5.3 OMNIS Software – Overview of functions

Functions with icons in the program as a whole

	Logged in user Display the currently logged in user in the tooltip. Further functions: **Lock OMNIS Software** or **Change password**.
•••	**Extras** 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.
	Saving Save all changes.

	Delete Delete the selected object.
	Update list Reload the view or list. All entries are reloaded. If there are unsaved changes, these will be discarded.
	Properties Open the **Properties** window to display and edit the settings of the currently selected object.
	Select view Open the selection list. Expand the selection list with various options for the field.
	Import Import the selected object.
	Export Export the selected object.
	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 (Comma Separated Value) file, saved to the selected file directory and deleted from the current database.
	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.
	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 a sample profile

Create a new sample profile to facilitate the entry of recurrent sample data.

(x)+ **Create system variable**

Create a new system variable for use throughout all commands, methods and operating procedures.

Functions with icons in the Sample list and / or Search queries subsection

	Selection for saving Select the required saving option from the selection list. **Save as new search query**: The filter criteria are saved as a new search query. **Save as new sample list**: The samples and subsamples that have been found with the filter criteria are saved as a new sample list.
	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.
	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 run test Assign work systems for the subsamples to be analyzed.
	Restore operating procedure and methods Restore the operating procedure and methods to the version they were in at the moment the subsample was executed.
	Single determination Analyze the highlighted subsample individually.
	Series determination Analyze all executable subsamples in the sample list sequentially.

	Parallel determination Analyze all executable subsamples in the sample list simultaneously.
	Start determination All subsamples that have not yet been processed are analyzed. In the single determination mode, only the selected subsample is analyzed.
	Stop determination immediately All running determinations are canceled.
	Stop determination after a delay The ongoing determination of the subsample is run until completion. Other determinations are not restarted.
	Add subsamples to sample series All additional subsamples are added to the running sample series and they are then analyzed.
	Remove subsamples from running sample series All highlighted subsamples are removed from the sample series currently running.
	Add to an ongoing 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 ongoing 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.

Functions with icons in the Processes work area

	Create operating procedure Create a new operating procedure in which methods (no editing) and commands can be inserted and edited.
	Create method Create a new method in which commands can be inserted and edited.
	Delete method Delete the method from the database. **Delete operating procedure** Delete the operating procedure. Methods contained in the operating procedure are retained in the database. Signed operating procedures or methods are locked and cannot be deleted.
	Edit tags Activate the editing of tags for the selected element.

Functions with icons in the Operating procedures and Methods subsections

	Library Open the **Library** window with the list of all available elements that can be inserted into operating procedures and methods.

Add report definition / export definition

Add report definition / export definition.

Remove report definition / export definition

Remove the defined report definition / export definition.

Validate the method

Check the assignments of functional units and work systems for correctness.

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.

Manual control

Open the **Manual control** window for the manual operation 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 prediction model

Create a new prediction model for calculating sample parameters from NIR spectra.

Slope/y-intercept correction

Create a new slope/y-intercept correction for the correction of the selected prediction model.

Delete prediction model

Delete the prediction model including published versions. Subsamples used in the prediction model are not deleted.

Delete slope/y-intercept correction

Delete the slope/y-intercept correction.

Functions with icons in the Prediction models and Slope/y-intercept corrections subsections

Publish

Publish the prediction model or the slope/y-intercept correction to be able to use it in determinations and repredictions.

Automatic splitting of data set

Opens the dialog for automatic splitting of the data set.

Add spectra

Add new spectra to the prediction model. Opens the dialog for selecting spectra from a sample list or search query.

Remove spectra

The spectra are removed from the prediction model.

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.

NOTICE

If the user management was activated with Active Directory integration, then no new users can be created and edited. New user accounts can be created and edited in Active Directory outside of the OMNIS Software and are added automatically to the OMNIS Software when the software is restarted.

Functions with shortcut keys

[F1]	**Open the help** Open OMNIS Help.
[CTRL]+[L]	**Lock OMNIS Software** Lock the OMNIS Software.
[CTRL]+[S]	**Saving** Save a sample list.
[CTRL]+[D]	**Duplicate** Duplicate selected sample list, operating procedure or method.
[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]	**Add** Add 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

Left mouse click	**Select object** Select the object.
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 required 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. ▪ On the **Methods** and **Operating procedure** tabs, the **Parameters** subsection in the **Properties** window is opened. ▪ In the overviews of the **Processes**, **Samples** and **Equipment** work areas, a new tab with the selected object is opened.

See also

Work system – Tab (chapter 5.2.7, page 110)

Operating procedure and method – Tab (chapter 5.2.6, page 108)

Sample list – Tab (chapter 5.2.3, page 100)

Sample profile – Tab (chapter 5.2.5, page 107)

Search query – Tab (chapter 5.2.4, page 104)

5.4 Locking or unlocking OMNIS Software

The OMNIS Software can be locked manually or automatically and thus protected against changes to the data.

NOTICE

Running processes are continued in the background.

Locking OMNIS Software manually

1 Locking manually

- Click on in the title bar of the OMNIS Software.
- Select **[Lock OMNIS Software]** in the selection list.
- Alternatively, lock the OMNIS Software with **[CTRL + L]**.

Locking OMNIS Software automatically

1 Activating automatic locking

- Activate 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.

After saving, the OMNIS Software is locked once the time has elapsed if no user activity (e.g. operating the keyboard or mouse) is registered.

Unlocking OMNIS Software

1 By the same user

- In the **Unlock OMNIS Software** window, enter the password and click on **[Unlock]**.

2 By another user

- Click on **[Switch user]** in the **Unlock OMNIS Software** window.
- In the **Log in to OMNIS Software** window, enter the **User ID** and the **Password** and click on **[Login]**.
- Click on **[Cancel]** in the **Log in to OMNIS Software** window to return the user to the **Unlock OMNIS Software** window where the previously logged in user can unlock the OMNIS Software.

NOTICE

The following is to be observed in the event of a login by another user:

- If a determination is running, then only users with the **Manage sample lists** right can log in.
- 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 activated, 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

User roles – Properties (chapter 4.6.7.1, page 60)

User roles – Directory (chapter 4.6.7.2, page 61)

User groups – Properties (chapter 4.6.6.1, page 56)

User groups – Definition (chapter 4.6.6, page 55)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (OMNIS) – Actions (chapter 4.6, page 23)

User rights – Directory (chapter 4.6.7.3, page 62)

User interface OMNIS Software – Overview (chapter 5.2, page 92)

5.5 Modification comment – Brief description

In **Settings ▶ Advanced settings**, under the option **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11**, if the **Modification comment** function is activated, the **Modification comment** dialog appears before saving the sample list. Before the modifications can be saved, a reason for the modification must be selected. Optionally, a comment can be entered for the change.

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

Setting up OMNIS Software (chapter 4.3, page 17)

User rights – Directory (chapter 4.6.7.3, page 62)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

5.6 Signature – Brief description

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 cannot be signed unless there are already signatures on level 1.
- 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/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

User rights – Directory (chapter 4.6.7.3, page 62)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

Setting up OMNIS Software (chapter 4.3, page 17)

Displaying a signature (chapter 5.6.2, page 134)

Creating a signature (chapter 5.6.1, page 132)

Deleting a signature (chapter 5.6.3, page 135)

Audit trail work area – Actions (chapter 5.12, page 917)

5.6.1 Creating a signature

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

NOTICE

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 *Editing a sample list (see chapter 5.8.1.2, page 143)*.

- 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

NOTICE

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).

NOTICE

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

User rights – Directory (chapter 4.6.7.3, page 62)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

Setting up OMNIS Software (chapter 4.3, page 17)

Signature – Brief description (chapter 5.6, page 131)

Deleting a signature (chapter 5.6.3, page 135)

Displaying a signature (chapter 5.6.2, page 134)

Audit trail work area – Actions (chapter 5.12, page 917)

5.6.2 Displaying a signature

Signature subsamples

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 Selecting the subsample

- Select the subsample for which the signature is to be shown.

3 Open a signature

- Open the **Subsample ▶ Signatures** subsection.

The signature for the selected subsample is displayed.

Signature operating procedures or methods

1 Selecting an operating procedure or method

- In **Processes ▶ Operating procedures** select the desired operating procedure which you require the signature to be shown for.
  or
- In **Processes ▶ Methods** select the desired method which you require the signature to be shown for.

2 Open a signature

- Click on to open the **Properties** window.

The signature for the selected operating procedure or method is displayed.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

Setting up OMNIS Software (chapter 4.3, page 17)

Signature – Brief description (chapter 5.6, page 131)

Creating a signature (chapter 5.6.1, page 132)

Deleting a signature (chapter 5.6.3, page 135)

Audit trail work area – Actions (chapter 5.12, page 917)

5.6.3 Deleting a signature

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

NOTICE

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 *Editing a sample list (see chapter 5.8.1.2, page 143)*.

- 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

NOTICE

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

NOTICE

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.

NOTICE

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

User rights – Directory (chapter 4.6.7.3, page 62)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (OMNIS) – Actions (chapter 4.6, page 23)

Setting up OMNIS Software (chapter 4.3, page 17)

Signature – Brief description (chapter 5.6, page 131)

Creating a signature (chapter 5.6.1, page 132)

Displaying a signature (chapter 5.6.2, page 134)

Audit trail work area – Actions (chapter 5.12, page 917)

5.7 Tags – Definition

Tags are used for categorizing and searching in overview lists. Operating procedures and methods can be organized according to tags without moving them into a folder. Multiple tags can be defined for each operating procedure or method. You can thus filter for tags in overview lists.

Those tags are retained during export, import or duplication.

See also

Creating and editing tags (chapter 5.7.1, page 137)

Filtering operating procedures and methods (chapter 5.9.1.4, page 270)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

5.7.1 Creating and editing tags

NOTICE

Newly created tags and any retrospective changes are applied immediately and are saved.

Creating and editing tags

1 Selecting an operating procedure or method

- In **Processes ▶ Operating procedures**, select an operating procedure to which a tag is to be added.
  or
- In **Processes ▶ Methods**, select a method to which a tag is to be added.

2 Activating the edit mode

- Activate the edit mode by clicking on .

The input field is opened.

3 Creating a new tag

- Write a new tag that does not exist yet into the input field and confirm with the **[Enter]** or **[Tabulator]** key.

NOTICE

Pay attention to the following when creating tags:

- All punctuation marks and numbers are permitted.
- 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 operating procedure or method, even if the use of upper and lower case differs.

The tag is created and is displayed in the input field as well as in the **Tags** column.

4 Selecting existing tags

- Click into the input field and select an existing tag in the selection list.
  or
  Write an existing tag into the input field. If the entry corresponds to a tag that already exists, then it can be selected in the selection list.
  or
  Click on the downwards **[arrow]** key, mark the desired tag and confirm with **[Enter]**.

NOTICE

You can select existing tags or recently used tags in the selection list.

5 Renaming tags

- Existing tags can be renamed by double-clicking on a tag or by pressing the **[backspace]** key. Confirm with **[Enter]** or **[Tab]** key.

NOTICE

The tag is renamed only in the selected method or operating procedure.

6 Deactivating edit mode

- Deactivate the edit mode by clicking on .

The input field is closed.

Remove tags

1 Remove individual tags

- Remove individual tags by clicking on in the tag.
- Alternatively, tags can also be removed with the **[Backspace]** key.

NOTICE

A tag is automatically deleted if it is no longer being used. However, the tag can be created again at any time.

2 Removing all tags

- Remove all tags in an operating procedure or method by clicking on in the input field.

See also

Operating procedure – Definition (chapter 5.9.1, page 260)

Filtering operating procedures and methods (chapter 5.9.1.4, page 270)

Method – Definition (chapter 5.9.2, page 281)

Tags – Definition (chapter 5.7, page 137)

Sorting the overview list (chapter 5.2.10, page 117)

5.8 Samples – Actions

You can execute the following actions in the subsections of the **Samples** work area:

- Samples and subsamples are selected, processed, signed or respectively locked and newly created in **Samples ▶ Sample lists**. The recorded subsamples can then be analyzed directly.
- 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**. Additionally, it is also possible to define how many subsamples are to be created automatically using which operating procedures.
- System variables are created, changed or deleted in a list in **Samples ▶ System variables**. System variables are variables that are defined across the system and that can be used in methods and operating procedures.

See also

Creating and deleting a sample list (chapter 5.8.1.1, page 142)

Creating and editing a sample profile (chapter 5.8.4.1, page 176)

Locking or unlocking samples (chapter 5.8.3.3, page 174)

Creating system variables (chapter 5.8.24.1, page 258)

Search queries – Definition (chapter 5.8.2, page 165)

Creating a signature (chapter 5.6.1, page 132)

Deleting a signature (chapter 5.6.3, page 135)

Sample list – Tab (chapter 5.2.3, page 100)

Sample profile – Definition (chapter 5.8.4, page 176)

System variables – Definition (chapter 5.8.24, page 257)

User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

User rights – Directory (chapter 4.6.7.3, page 62)

5.8.1 Sample lists – Subsection

The following functions are available in **Samples ▶ Sample lists**:

- With **Create sample list**, a new sample list is created in which samples and subsamples can be inserted and edited.
- With **Duplicate sample list**, the selected sample list is duplicated under the same name, at which time an index is also inserted after the name. 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 list contains duplicates of the samples and subsamples from the original sample list. The subsamples have the **Ready** status and can be analyzed immediately.
- With **Archive samples from sample list**, the samples in the selected sample list are archived along with their subsamples. The samples in the selected sample list are archived along with their subsamples. They are deleted from the database. The sample list is also deleted.
- With **Delete sample list**, the selected sample list is deleted. 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.

See also

Sample list – Tab (chapter 5.2.3, page 100)

Editing a sample list (chapter 5.8.1.2, page 143)

5.8.1.1 Creating and deleting a sample list

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 registration card.

3 Saving

- Enter samples or subsamples in the sample list*Creating samples (see chapter 5.8.3.1, page 171)*.
- Save the created sample list by clicking on .

Deleting a sample list

1 Selecting a sample list

- In **Samples ▶ Sample lists**, select the desired sample list.

2 Deleting a sample list

- Click on to delete the selected sample list.

NOTICE

The samples and subsamples contained in the sample list are retained in the database when the sample list is deleted and are thus also retained in other sample lists.

See also

Editing a sample list (chapter 5.8.1.2, page 143)

Creating samples (chapter 5.8.3.1, page 171)

Recording subsamples (chapter 5.8.5.1, page 181)

5.8.1.2 Editing a sample list

NOTICE

Save all changes in the sample list by clicking on . All unsaved changes are lost.

Renaming a sample list

1
- Enter the desired name in **Samples ▶ Sample list** in the **Name** field.
- Confirm the entry by clicking **[Enter]**.

The new name is automatically entered in the tab.

Adding samples or subsamples

1 Add a sample

- Select the appropriate sample profile in the selection list.
- To add a sample at a particular position in the sample list, click to select the sample under which the new sample is to be added.
- 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.

2 Add a subsample

- Click to select the subsample under which the new subsample is to be added.
- Add an additional subsample to the selected sample by clicking **+**. The operating procedure is taken over automatically from the preceding subsample.

Selecting the sample or subsample

1 Selecting individual samples or subsamples

- Click on or to select individual samples or subsamples.
- Click on or to select all samples or subsamples of a group.

2 Selecting multiple samples or subsamples

- To select multiple samples or subsamples, click the required samples or subsamples while pressing down the **[CTRL]** key.
- To select an entire area, select the first value with the left mouse button and, while holding the **[SHIFT]** key pressed down, click the last value of the section.

NOTICE

If a sample or multiple subsamples are selected, then clicking another sample or subsample while holding the **[CTRL]** key and **[SHIFT]** key pressed down will select all of the cells that lie in between.

NOTICE

If a sample or multiple subsamples are selected, then individual samples or subsamples can be deselected again with one click while holding the **[CTRL]** key pressed down.

If a sample or multiple subsamples are selected, then clicking another sample or subsample while holding the **[CTRL]** key and **[SHIFT]** key pressed down will deselect all cells that lie in between.

Selecting cells in the sample list

1 Selecting individual cells

NOTICE

Only cells within the same column can be selected together.

- If a cell is selected, then additional cells with the same name and type can be added to the selection with one click while holding the **[CTRL]** key pressed down.
- If a cell is selected, then clicking a different cell with the same name and type while holding the **[SHIFT]** key pressed down causes all of the cells in between to be added to the selection.

2 Selecting and deselecting multiple cells

- If multiple cells are selected, then clicking a different cell with the same name and type while holding the **[CTRL]** key and **[SHIFT]** key pressed down causes all of the cells in between to be selected.
- If multiple cells are selected, then clicking individual cells while holding the **[CTRL]** key pressed down causes those cells to be deselected again.
- If multiple cells are selected, then clicking a different cell with the same name and type while holding the **[CTRL]** key and **[SHIFT]** key pressed down causes all of the cells in between to be deselected.

Editing cells in the sample list

1 Editing content

- Double-click a cell within the sample list.

Incrementing cells in a column

Prerequisite:

- The topmost cell contains a number.

1 Selecting a cell

- Select the desired cells within a column.

2 Incrementing content

- Right-click on one of the cells to open the context menu.
- Select the **Increment** function.

The numerical value of the selected cell at the top is taken as base value for incrementing the selected section.

Filling cells in a column

Prerequisite:

- The topmost cell contains a number or a text.

1 Selecting a cell

- Select the desired cells within a column.

2 Filling content

- Right-click on one of the cells to open the context menu.
- Select the **Fill** function.

The content of the topmost selected cell is inserted into the other cells of the selected area.

Cutting and pasting samples or subsamples

Prerequisite:

- A sample or a subsample is selected: *(see "Selecting the sample or subsample", page 143)*.

1 Cutting the sample or subsample

- Open the context menu by right-clicking the highlighted section and select **[Cut]**.

NOTICE

Multiple samples and subsamples can be cut and pasted.

2 Inserting a 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]**.

NOTICE

During the run, the inserted subsamples are executed in their new position in the sample list. This allows individual subsamples to be prioritized.

Removing samples and subsamples

Prerequisite:

- A sample or a subsample is selected: *(see "Selecting the sample or subsample", page 143)*.

1 Removing sample or subsample

- Click or to remove the selected sample or subsample from the list.
- To remove samples and subsamples from the sample list, right-click a highlighted sample or subsample to open the context menu and select **[Remove from sample list]**.

NOTICE

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 samples or subsamples

Prerequisite:

- A sample or a subsample is selected: *(see "Selecting the sample or subsample", page 143)*.

1 Deleting the sample or subsample

- Right-click on the selected sample or subsample to open the context menu.
- Select **[Delete]** in the context menu.

NOTICE

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.

The sample or subsample is deleted.

Adding sample data

Prerequisite:

- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*.

1 Opening the "Adding sample data" dialog

- 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 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.
- In the **Type of input field** field, select the desired type (**Text**, **Number** or **Selection list**).

- Select the desired 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 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.
- Activate the **Editable field** check box if the input field for the sample in the sample list is to be available for editing.

NOTICE

The option of marking a field as editable or the entire **Properties input field** section is not available in the following cases:

- If **Text** or **Number** was selected in **Type of input field** while at the same time **Result** was selected in **Use as**.
- If **Selection list** was selected in **Type of input field**.

NOTICE

Sample data can also be defined in Sample profile. Sample data that is recorded directly in the sample list do not however have an influence on the sample data in the sample profile being used. Additional information on the sample profile: *Creating and editing a sample profile (see chapter 5.8.4.1, page 176)*

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]**.

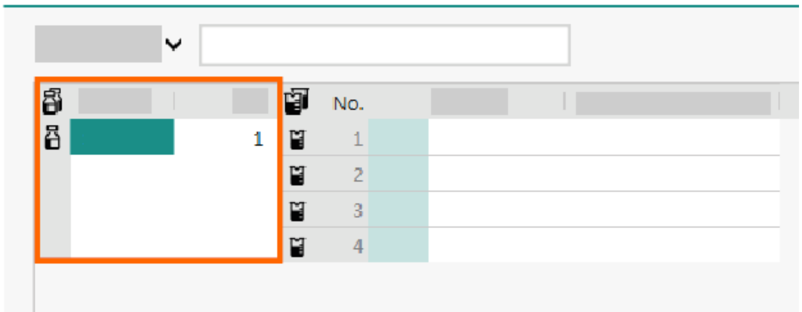
4 Modifying the sequence of sample data (optional)

- Select the desired 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 yet been analyzed.

Updating the sample list

1 Updating the sample list

- Update the sample list including all sample data and subsample data by clicking or **[F5]**.

NOTICE

Unsaved changes are lost when the sample list is updated.

See also

Creating and deleting a sample list (chapter 5.8.1.1, page 142)

Creating samples (chapter 5.8.3.1, page 171)

Recording subsamples (chapter 5.8.5.1, page 181)

Importing subsample data (chapter 5.8.5.6, page 197)

Exporting subsample data (chapter 5.8.1.3, page 151)

Samples – Actions (chapter 5.8, page 140)

Creating a report (chapter 5.8.1.5, page 159)

Run test – Brief description (chapter 5.8.6.1, page 199)

Subsamples – Statuses (chapter 5.8.5.2, page 184)

Creating and editing a sample profile (chapter 5.8.4.1, page 176)

Signature – Brief description (chapter 5.6, page 131)

5.8.1.3 Exporting subsample data

There are 3 options in the OMNIS Software for exporting subsample data:

- *Automated export* during a determination with the **EXPORT** command *EXPORT – Parameters (see chapter 5.9.4.16.4, page 593)*.
- *Automated export* after a determination has been run. The setting can be made under **Processes ▶ Operating procedures ▶ Properties ▶ Exports**.
- *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.

NOTICE

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 by the "**;**" character.

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 target folder path directly to which the CSV file is to be saved.
- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

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 desired 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.

The exports can be defined in **Properties ▶ Exports**.

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**.
- Select a target folder by clicking in the **Target folder** field. Alternatively, enter the target folder path in which the export is to be saved.
- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

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**.
- Select a target folder by clicking in the **Target folder** field. Alternatively, enter the target folder path in which the export is to be saved.
- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

4 Creating an export file

- Click on **[Export]** to create the export file.

NOTICE

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**).

5 Opening the target folder

- Click **[Open target folder]** to open the directory with the created files.

See also

Recording subsamples (chapter 5.8.5.1, page 181)

Importing subsample data (chapter 5.8.5.6, page 197)

5.8.1.4 Report template – Directory

The following report templates are available for creating reports using the **REPORT** command, an operating procedure or from the sample list:

NOTICE

Further information on creating reports: *Creating a report (see chapter 5.8.1.5, page 159)*

Name	Content
Calibration report	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
Sample result report Sample result report (short)	Results, including curves and data, of all subsamples of a sample. 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 ***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 ▪ Operating procedure used

Name	Content
Subsample equipment report	Data regarding all of the work systems, functional units and accessories used for carrying out the subsample. Data concerning the following is listed therein: ▪ Subsample ▪ Instrument ▪ Work systems with 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:
	▪ Subsample
	▪ Operating procedure
	▪ Signatures
	▪ Subsample data
	▪ Monitoring
	▪ Methods and commands
	  – Method
	  – Work systems
	  – Signatures
	▪ Commands with work systems

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
	Note: The conditioning curve and conditioning data of the **COND CHECK** command are not displayed in the **Subsample result report (short)**.

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. Further information in: *EXPORT – Parameters (see chapter 5.9.4.16.4, page 593)*. ***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** and **Models**, the possibility also exists of creating reports directly. The following report types are available:

Name	Content
Parameter 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
Parameter report – Method	Parameters of a selected method. Data concerning the following is listed therein: ▪ Method ▪ Signatures ▪ Work systems ▪ Method variables ▪ Commands with work systems
Report – Prediction model	Parameters and data of a selected prediction model. Data concerning the following is listed therein: ▪ Prediction model type full ▪ Properties ▪ Prediction model type light ▪ Wavelength range ▪ Data preprocessing ▪ Figures of merit ▪ Correlation plot ▪ Spectra list
Report – slope/y-intercept correction	Parameters and data of a selected slope/y-intercept correction.

See also

Operating procedure – Properties (chapter 5.9.1.2, page 262)

Audit trail work area – Actions (chapter 5.12, page 917)

User rights – Directory (chapter 4.6.7.3, page 62)

Setting up a printer (chapter 5.13.1, page 932)

EXPORT – Parameters (chapter 5.9.4.16.4, page 593)

REPORT – Parameters (chapter 5.9.4.16.11, page 607)

Creating a report (chapter 5.8.1.5, page 159)

Exporting subsample data (chapter 5.8.1.3, page 151)

5.8.1.5 Creating a report

The following options for creating reports are available in the OMNIS Software:

- *Automated report creation* during a determination with the **REPORT** command *REPORT – Parameters (see chapter 5.9.4.16.11, page 607)*.
- *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**.

Automated report creation with the REPORT command

1 Inserting a 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 the 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 a report

- Select the desired report template in the **Report template** field *Report template – Directory (see chapter 5.8.1.4, page 155)*.
- Select the desired output language in the **Output language** field.
- Select the output format **PDF file** or **Paper printout**.
- Select a target folder by clicking on in the **Target folder** field. Alternatively, enter the target folder path in which the report is to be saved. If the defined folder does not exist, it is created when creating the report.
- Enter the name under which the file is to be saved in the **PDF file name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

4 Saving the report

- Save the report by clicking on .

Automated report creation from the operating procedure

1 Opening an operating procedure

- In **Processes ▶ Operating procedures**, select the desired operating procedure and open it with a double-click.

2 Opening the reports

- Click on to open the **Properties** window.
  or
- Double-click on the operating procedure icon to open the **Properties** window directly.
- Open the **Properties ▶ Reports** subsection.

3 Adding a report

- Click on to add a new report.

4 Defining a report

- Select the desired report template in the **Report template** field *Report template – Directory (see chapter 5.8.1.4, page 155)*.
- Select the desired output language in the **Output language** field.
- Select the output format **PDF file** or **Paper printout**.
- Select a target folder by clicking on in the **Target folder** field. Alternatively, enter the target folder path in which the report is to be saved. If the defined folder does not exist, it is created when creating the report.
- Enter the name under which the file is to be saved in the **PDF file name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

5 Saving the report

- Save the report by clicking on .

Manual report creation from the sample list

1 Selecting samples or subsamples

- Reports for selected 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.
- Click and select **Selected subsamples**.
  or
- Reports for all subsamples in the sample list:
  Click and select **All subsamples in the list**.

> **NOTICE**
>
> A report is created for each of the selected samples or subsamples.

2 Defining a report

- Select the desired report template in the **Report template** field *Report template – Directory (see chapter 5.8.1.4, page 155)*.
- Select the desired output language in the **Output language** field.
- 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 defined folder does not exist, it is created when creating the report.
  - Enter the name under which the file is to be saved in the **PDF file name** field.
  - Create the PDF file by clicking on **[Create PDF]**.

  or
- Select the **Paper printout** output format.
  - Create the report by clicking on **[Print]**.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

Manual report creation from the work area Processes

1 Selecting an operating procedure or method

- Select the desired operating procedure in **Processes ▶ Operating procedures**.
  or
- Select the desired method in **Processes ▶ Method**.
- Click on to open the window to enter the file name and the target folder.

A new windows opens.

2 Defining file names and target folders

- Enter the name under which the file is to be saved in the **PDF file name** field.
- Select the target folder or enter the absolute path in the address bar that the exported file is to be saved to.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

3 Creating a report

- Create the report by clicking on **[Save]**.

Manual report creation from the work area Models

1 Selecting the prediction model or slope/y-intercept correction

- Select the desired prediction model in **Models ▶ Prediction models**.
  or
- Select the desired slope/y-intercept correction in **Models ▶ Slope/y-intercept corrections**.
- Click on 🗎 to open the window to enter the file name and the target folder.

A new windows opens.

2 Defining file names and target folders

- Enter the name under which the file is to be saved in the **PDF file name** field.
- Select the target folder or enter the absolute path in the address bar that the exported file is to be saved to.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

3 Creating a report

- Create the report by clicking on **[Save]**.

Applying a custom logo

The Metrohm logo is inserted as a logo on the top left corner of the report by default. You can use your own logo by replacing the **logo.png** file in the OMNIS installation directory under "**...\Metrohm\Desktop\Resources\ReportTemplates**". You need local administrator rights to be able to make changes in this directory.

The new file must fulfil the following points to be detected by the software:

- File format: BMP, JPG, PNG, TIFF
- File name: **logo.*** (* = bmp, jpg, png, tiff)

NOTICE

- 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 5.9.1.3, page 265)

Setting up a printer (chapter 5.13.1, page 932)

REPORT – Parameters (chapter 5.9.4.16.11, page 607)

Report template – Directory (chapter 5.8.1.4, page 155)

5.8.2 Search queries – Definition

All saved **search queries** are displayed in **Samples ▶ Search queries**. Search queries are **Sample lists**, that are compiled dynamically. A search query defines the filter criteria with which the database is searched.

NOTICE

Search queries that are open cannot be deleted.

See also

Samples – Actions (chapter 5.8, page 140)

Creating a Search queries (chapter 5.8.2.2, page 166)

Filtering Search queries (chapter 5.8.2.3, page 167)

Sample list – Tab (chapter 5.2.3, page 100)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Sorting the overview list (chapter 5.2.10, page 117)

5.8.2.1 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.
- **Delete search query** deletes the search query. 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 modified after opening the search query.
Saved	Time at which the search query was last saved.

See also

Search queries – Definition (chapter 5.8.2, page 165)

Creating a Search queries (chapter 5.8.2.2, page 166)

Filtering Search queries (chapter 5.8.2.3, page 167)

Search query – Tab (chapter 5.2.4, page 104)

5.8.2.2 Creating a Search queries

Create a search query

1 Setting up search queries

- Click on in **Samples ▶ Search queries**.

A new tab opens with **New search query** as its title.

2 Naming a search query

- Enter the desired name in the name field for the new search query and confirm with **[Enter]**.

3 Saving a search query

- Save the search query by clicking on .

The name entered is displayed on the registration card.

Save as new search query / sample list

1 Click on ✓ and select the **Save as new search query** option to save the configured filter criteria as a new search query.

2 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.

The samples and subsamples can then be processed as usual.

NOTICE

Samples and subsamples can be deleted in the **Search queries** subsection *Editing a sample list (see chapter 5.8.1.2, page 143)*.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Search queries – Definition (chapter 5.8.2, page 165)

Filtering Search queries (chapter 5.8.2.3, page 167)

Sample list – Tab (chapter 5.2.3, page 100)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

5.8.2.3 Filtering Search queries

- With the **Monitoring status** filter criterion, the results of the result monitoring can be found under **Samples ▶ Sample list ▶ Results ▶ Monitoring**. Further information: *Filtering the monitoring status (see chapter 5.8.22.2, page 253)*
- 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**. Further information: *Sample list – Tab (see chapter 5.2.3, page 100)*
- With the **Calculation result** filter criterion, invalid results from the **Result value** column can be found under **Samples ▶ Sample lists ▶ Results ▶ Calculations**. Further information: *Calculations – Definition (see chapter 5.8.19, page 243)*

1 **Opening a search query**

- In **Samples ▶ Search queries**, select the desired search query and open it with a double-click.

2 Opening filters

- Open the filter by clicking on .

The area for selecting configurable filter criteria is opened.

3 Selecting a 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 a filter criterion

- Add the filter criterion by clicking on .

NOTICE

Any number of filter criteria can be added to refine the search.

5 Selecting the filter criterion

- Select a filter criterion from the selection list.

NOTICE

Depending on the filter criterion, a variety of search operators and options to choose from are available.

6 Selecting a search operator

Select a search operator from the selection list.

- **Contains**
  – The search results contain the entered object.
- **Equals**
  – The search results exactly match the entered object.
- **Does not equal**
  – The search results do not match the entered object.

7 Limiting the filter criterion

- If necessary, enter or select a search term, the number of days, values or a date, depending on the filter criterion that was selected beforehand.

8 Filtering

- Apply the selected filter criteria by clicking on **[Filter]**.

The results are displayed in the list according to the filter criteria.

9 Limiting the results

- Select the number of entries (e.g. 10 entries) in the selection list.

The number of entries is displayed according to the selection in the list.

10 Selecting the 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.

NOTICE

If samples or subsamples in a sample list have been changed in the meantime, click on ⟳ to update the list.

In addition, the filter is reapplied when the pages are changed.

11 Resetting filters

- 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.

12 Removing filter criterion

- Remove the filter criterion by clicking on ✕.

> **NOTICE**
>
> If a filter criterion is deleted, then the filter needs to be applied again to see the corresponding entries.

13 Close filters

- Click on ▼ or ↑ to close the filter.

> **NOTICE**
>
> The filter criteria remain active, even after closing the filter.

The area for selecting configurable filter criteria is closed.

14 Saving a search query

- Changes are saved by clicking on 💾.

> **NOTICE**
>
> The configured filter criteria can also be saved as a new search query or sample list by clicking on ⌄*Creating a Search queries (see chapter 5.8.2.2, page 166)*.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Calculations – Definition (chapter 5.8.19, page 243)

Sample list – Tab (chapter 5.2.3, page 100)

Search queries – Definition (chapter 5.8.2, page 165)

Creating a Search queries (chapter 5.8.2.2, page 166)

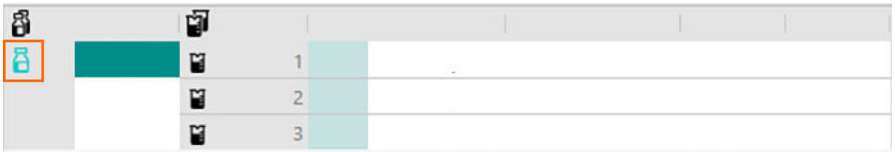
Filtering the monitoring status (chapter 5.8.22.2, page 253)

5.8.3 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 samples (chapter 5.8.3.1, page 171)

Creating and editing a sample profile (chapter 5.8.4.1, page 176)

5.8.3.1 Creating samples

Prerequisite:

- To add a sample to the sample list, you must have created a sample profile beforehand.

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 Add new sample

- Click +.

A new sample is created with the number of subsamples defined in the sample profile.

NOTICE

If the sample is created without a sample profile, then a minimum sample profile with a column header (**Sample name**) will be used for the sample by default. The subsample must be added manually to the sample in such cases.

3 Entering sample data

- Enter or supplement the sample data as needed.

4 Saving sample data

- Save the sample data.

NOTICE

Click to remove a sample from the sample list once again. Sub-samples that have already been recorded will also be removed at this time.

The sample is not deleted from the database. If this is desired, press **[CTRL]**+**[DEL]** or click the sample with the right mouse button and select **[Delete]**.

See also

Creating and editing a sample profile (chapter 5.8.4.1, page 176)

Sample list – Tab (chapter 5.2.3, page 100)

Recording subsamples (chapter 5.8.5.1, page 181)

5.8.3.2 Archiving samples

NOTICE

By archiving samples, the size of the database can be effectively reduced and storage space can be saved.

Prerequisite:

- The user has the **Archive samples** right.
- The **Sample lists** subsection is opened.

1 Archiving the sample list

- Select the sample list for which the samples and subsamples are to be archived under **SamplesSample lists**.
- Start archiving by clicking on and continue the process by clicking on **[Archive]**.

A new windows opens.

NOTICE

Sample lists that are open and have not been saved are not archived.

2 Selecting or entering a 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.

NOTICE

If a new folder is created, the following special characters or character strings may not be used:

>, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

3 Creating an archive file

- Click on **[Select folder]**.

The samples in the selected sample list are archived along with their subsamples and an entry for the steps of the process is created in the audit trail. The OSIN files are exported to and saved in the target folder. The samples are deleted from the database. The sample list is also deleted.

NOTICE

This may take several minutes.

Subsamples of a sample that is to be archived that are in another sample list are also archived and subsequently will no longer be displayed in the other sample list.

All time indications are converted into the 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.

For the date and time displayed in the file name, the local time on the computer is used.

See also

Exporting operating procedure and method (chapter 5.9.1.6, page 272)

Audit trail work area – Actions (chapter 5.12, page 917)

Archiving the audit trail (chapter 5.12.5, page 928)

User rights – Directory (chapter 4.6.7.3, page 62)

Exporting subsample data (chapter 5.8.1.3, page 151)

5.8.3.3 Locking or unlocking samples

NOTICE

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

NOTICE

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 *Editing a sample list (see chapter 5.8.1.2, page 143)*.

- 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

NOTICE

Samples can be multi-selected *Editing a sample list (see chapter 5.8.1.2, page 143)*.

- Right-click the selected samples and select **[Unlock]** in the context menu.

The samples are unlocked.

See also

Setting up OMNIS Software (chapter 4.3, page 17)

User rights – Directory (chapter 4.6.7.3, page 62)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

Editing a sample list (chapter 5.8.1.2, page 143)

Audit trail work area – Actions (chapter 5.12, page 917)

5.8.4 Sample profile – Definition

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 a sample profile (chapter 5.8.4.1, page 176)

5.8.4.1 Creating and editing a sample profile

Prerequisite:

- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Creating a sample profile

- In **Samples ▸ Sample profiles**, click on **+**.

A new tab opens with **New sample profile** as its title.

NOTICE

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 a sample profile

- Enter the desired name in the **Sample profile name** field.

After confirmation with **[Enter]**, the new name is entered on the tab automatically.

3 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.

NOTICE

To delete sample data, right-click in the text field and select **[Delete input field]**.

NOTICE

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: *Editing a sample list (see chapter 5.8.1.2, page 143)*

4 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.

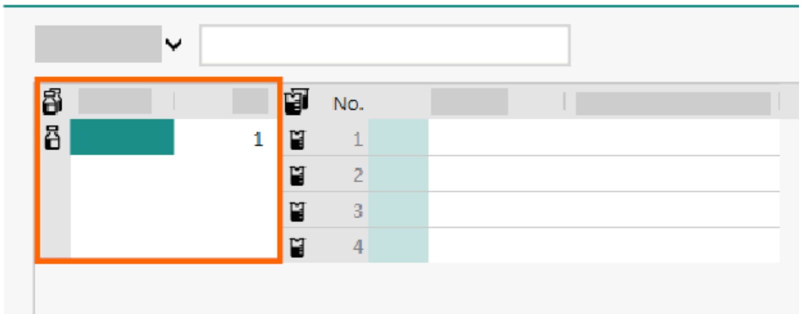
- Enter the name for the input field that is to be used as designation in reports in the **Field name long** field for each new entry. ***Note:*** If no name is entered in the **Field name long** field, then the name in the **Field name short** field will be used in the reports.
- Select the desired type (**Text**, **Number** or **Selection list**) for the information in the **Type of input field** field.
- Select the desired 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**).
- 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**
- Activate the **Editable field** check box if the user should be able to edit the input field for the sample in the sample list.

NOTICE

The option of marking a field as editable or the entire **Properties input field** section is not available in the following cases:

- If **Text** or **Number** was selected in **Type of input field** while at the same time **Result** was selected in **Use as**.
- If **Selection list** was selected in **Type of input field**.

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.



In addition, the sample data (with exception of the **Name** field) is also available as variables with the respective names in the formula editor.

NOTICE

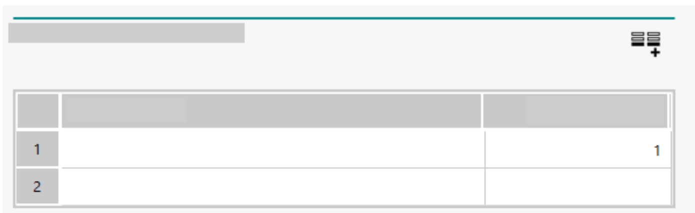
To delete an input field, right-click the name field and select **[Delete input field]**.

5 Modifying the sequence of sample data (optional)

- Select the desired input field by clicking an editable field and move it to the left by clicking or move it to the right by clicking .

6 Defining the operating procedure and the number of subsamples

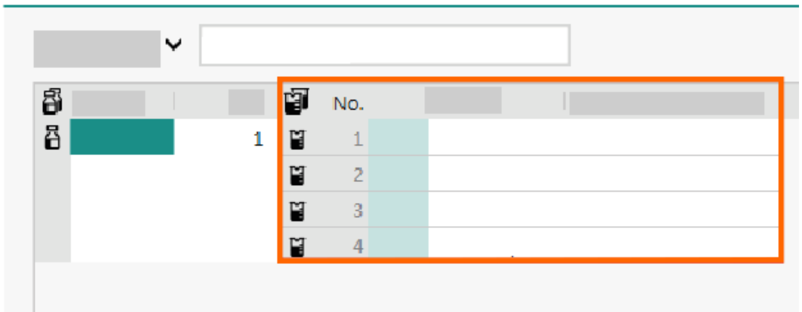
- In the **Operating procedures / subsamples** area, define the operating procedures and the associated number of subsamples that are added automatically to the sample list along with the sample data.
  To add a new line, right-click in the table and select **[Add new row]** or click on .



NOTICE

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.

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.



NOTICE

To delete a line, right-click on the selected table row and select **[Delete row]**.

7 Saving a sample profile

- Save the sample profile by clicking on .

See also

Sample profile – Definition (chapter 5.8.4, page 176)

Creating samples (chapter 5.8.3.1, page 171)

5.8.5 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

Recording subsamples (chapter 5.8.5.1, page 181)

Editing subsample data (chapter 5.9.1.8.1, page 275)

5.8.5.1 Recording subsamples

Recording subsamples in the sample list

Prerequisite:

- A sample profile has been created. *Creating and editing a sample profile (see chapter 5.8.4.1, page 176)*
- The user has the **Manage samples** or **Edit samples/not analyzed subsamples** right.
- A sample list is opened and at the front.

NOTICE

If no sample profile or 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.

1 Selecting a sample (optional)

- Select the sample to which a subsample is to be added.

2 Adding a subsample

- Add a new subsample by clicking on +.

The new subsample is added to the sample list below the subsamples of the selected sample that are already present. The focus switches automatically to the newly added subsample.

3 Naming a subsample

- Double-click in the **Subsample name** field and enter the desired name.

NOTICE

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. By default, the operating procedure that has the subsample above the newly inserted subsample is selected.

5 Editing additional subsample data

- Double-click in the desired field and edit the content.

6 Saving the sample list

- Save the sample list by clicking on .

Inserting a subsample between other subsamples

Prerequisite:

- The user has the **Manage samples** or **Edit samples/not analyzed subsamples** right.
- A sample list is opened and at the front.
- There are several samples and subsamples in the sample list.

1 Selecting a subsample

- Select the subsample after which a new subsample is to be added.

2 Adding a subsample

- Add a new subsample by clicking on .

The subsample is added after the selected subsample and highlighted automatically. The operating procedure is adopted by the selected subsample, but the rest of the subsample data is not, however.

3 **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.

Depending on which subsample data the newly determined operating procedure brings with it, it may happen that, due to different subsample data, a new line with different column headers will be inserted.

Adding an additional subsample to a running sample series

Prerequisite:

- A sample series is already being run in a sample list.
- Further samples and subsamples should be added to the sample series.

1 **Adding samples or subsamples to the sample list**

- Add a new sample to the sample list by clicking on .
  or
- Add a new subsample to the selected sample by clicking on .
- Edit the sample data and subsample data of the new subsample.
- Save the sample list by clicking on .

2 **Adding samples or subsamples to the ongoing sample series**

- All new samples and subsamples: All newly recorded and saved samples and subsamples for the current sample series can be added by clicking on . They are executed according to their position in the sample list.
  or
- Individual samples: Click on to select the individual samples. Right-click on the status field of a highlighted subsample to open the context menu and click on .
- or
- Individual subsamples: Click on or on the status field of a subsample to select the desired subsample. Right-click or left-click on the status field to open the context menu and click on .

During the series determination, subsamples that are added below the currently running subsample are processed according to the order of execution, from top to bottom. Subsamples that are inserted above the currently running subsample are executed after the determination of the last subsample at the bottom of the sample list.

See also

Operating procedure – Definition (chapter 5.9.1, page 260)

Starting a determination (chapter 5.8.6.6, page 207)

Stopping a determination (chapter 5.8.6.7, page 209)

Creating samples (chapter 5.8.3.1, page 171)

Sample list – Tab (chapter 5.2.3, page 100)

Editing subsample data (chapter 5.9.1.8.1, page 275)

5.8.5.2 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.

NOTICE

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

Status field	Meaning	Possible status changes
	Work system ready The work system used for the subsample is in the Conditioning OK status.	No status change possible
	Work system not ready The work system used for the subsample is in the Conditioning not OK status.	No status change possible
	Held The analysis of the subsample was held.	Continue determination Stop determination
	Waiting for user action The analysis of the subsample was held. The execution is continued as soon as data from an RS-232 interface has been received or entered manually in the **Live data** subsection of the **Curves and data** area.	Stop determination
	Waiting for work system The analysis of the subsample was held. The work system required for the determination is faulty or currently in use.	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

Status field	Meaning	Possible status changes
	Reprocessed, not saved The data of the analysis was modified retroactively, but not yet saved.	No status change possible

See also

Editing a sample list (chapter 5.8.1.2, page 143)

Pausing a determination (chapter 5.8.6.8, page 209)

5.8.5.3 Carrying over weighing data to subsamples

If a balance is connected to the OMNIS system, the weight and weight units can be carried over directly into a sample list.

NOTICE

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: *Operating the Cubis II balance (see chapter 5.10.1.16, page 682)*

Carrying over weighing data

A weight and the corresponding unit can be added to the subsample data with a **WEIGH** command, a **REQUEST** command or by pressing the **[Print]** key on the balance.

Editing subsample data (see chapter 5.9.1.8.1, page 275)

Prerequisites:

- 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**:*Configuring the balance (see chapter 5.10.1.15, page 680)*

Carrying over weighing data directly

1. 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. Weigh in the subsample at the balance.
3. On the balance, press the **[Print]** key.

Carrying over weighing data with the WEIGH command

Prerequisites:

- 2 input fields of the **Result** type must be defined in the parameters of the operating procedure; one for the weight and the other for the result.

1 Create a method with a **WEIGH** command and 2 **CALC** commands.

2 Add the following entries in the parameters of the **CALC** command to carry over the weight:

- Select the '**Weigh.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 Add the following entries in the parameters of the second **CALC** command to carry over the unit:

- Select the '**Unit.Result**.*Command name*' variable in the **Formula** field under **Command variables**.
- Select the second variable '*Variable name*.**CurrentSubsample-Data**' in the **Save result in variable** field under **Subsample data**.

4 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, this will also be signaled by an acoustic signal.

Carrying over weighing data by weighing by difference

Prerequisites:

- An input field of the **Sample size** type must be defined in the parameters of the operating procedure.
- The execution of the subsample with a **REQUEST** command must be ongoing and the **REQUEST** window must be open.

- The weighing data can be changed as long as the **REQUEST** window is open. It can subsequently only be changed if the **Editable field** option was activated when the input field was defined in the operating procedure.

1 To change the unit, activate the check box **Edit unit** in the parameters of the **REQUEST** command.

2 Weigh the subsample at the balance and then tare the balance.

3 Once the **REQUEST** command is displayed, add the sample and place the empty weighing vessel back on the balance.

4 On the balance, press the **[Print]** key.

5 Click **[Continue]**.

The values for the running subsample are applied.

NOTICE

Applying the weighing data works only if the sample list is opened and the **REQUEST** window is open. If another work area or another tab in the **Samples** work area is opened, then the data sent by the balance is not applied.

See also

Configuring the balance (chapter 5.10.1.15, page 680)

Editing subsample data (chapter 5.9.1.8.1, page 275)

5.8.5.4 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.

NOTICE

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.

NOTICE

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 5.9.1.3, page 265)

Recording subsamples (chapter 5.8.5.1, page 181)

Subsamples – Statuses (chapter 5.8.5.2, page 184)

Reprocessing calculations (chapter 5.8.19.1, page 244)

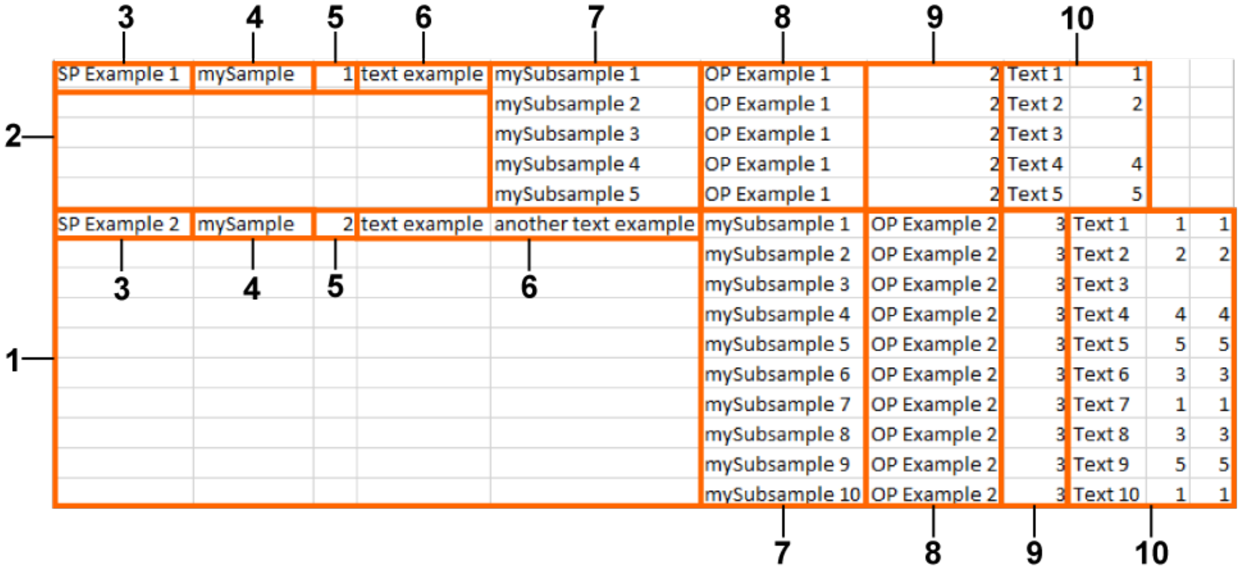
Creating and editing a sample profile (chapter 5.8.4.1, page 176)

5.8.5.5 Preparing a CSV file

CSV files can be used to import and export subsample data (e.g. sample lists from a third-party system). For the import, the file should be prepared correctly. For the export, individual options in the Windows system settings may have to be changed.

NOTICE

To ensure that the required decimal separator is used, the regional format must be changed: *(see "Configuring the decimal separator", page 196)*



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

1 **Sample 1**
Multiple samples and subsamples can be imported in a file.

2 **Sample 2**
Multiple samples and subsamples can be imported in a file.

3 **Name of the sample profile**
The sample profile listed in the CSV file must exist under the identical name in the OMNIS Software.

4 **Sample name**
The sample name can be freely assigned. The following characters are not allowed: **.|'"{}**

5 **Number of additional sample data**
The maximum number of sample data in the CSV file must not exceed the number of sample data that was defined 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**
The number and type of the field are defined in the sample profile.

7	**Subsample names** The subsample names can be freely assigned. The following characters are not allowed: **.|'"{}**	**8**	**Name of the operating procedure** The operating procedure listed in the CSV file must exist under the identical name in the OMNIS Software.
9	**Number of additional subsample data** The maximum number of subsample data in the CSV file must not exceed the number of subsample data that was defined in the operating procedure. 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** The number and type of the field are defined in the sample profile:

NOTICE

Example of a CSV file with sample data and subsample data: *Knowledge Base*

NOTICE

A CSV file can be edited, e. g. in Microsoft Excel. To accomplish this, an XLSX file is created and saved as a CSV file in the last step.

Preparing a CSV file

1 Opening CSV files in the table editing program

```
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
```

- 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.

2 Creating an operating procedure in OMNIS Software

- Create a new operating procedure under **Processes ▶ Operating procedures**.
- Enter the name of the operating procedure under **Properties ▶ General**.

NOTICE

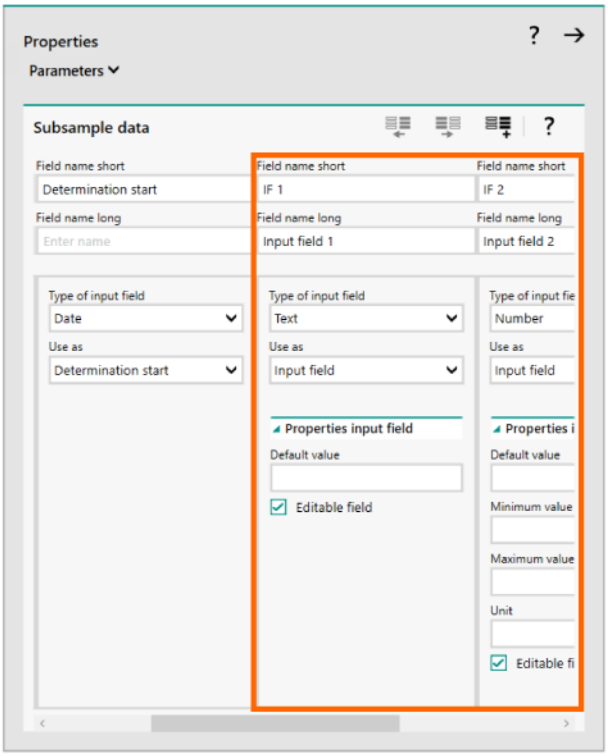
The following characters are not allowed: **.|'"{}**

NOTICE

Further information on creating an operating procedure: *Creating and editing an operating procedure (see chapter 5.9.1.3, page 265)*

3 Defining subsample data

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



- 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 in accordance with the data in the CSV file.
  - The **Editable field** check box is activated.

NOTICE

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.

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 **Sample profile name** field.

NOTICE

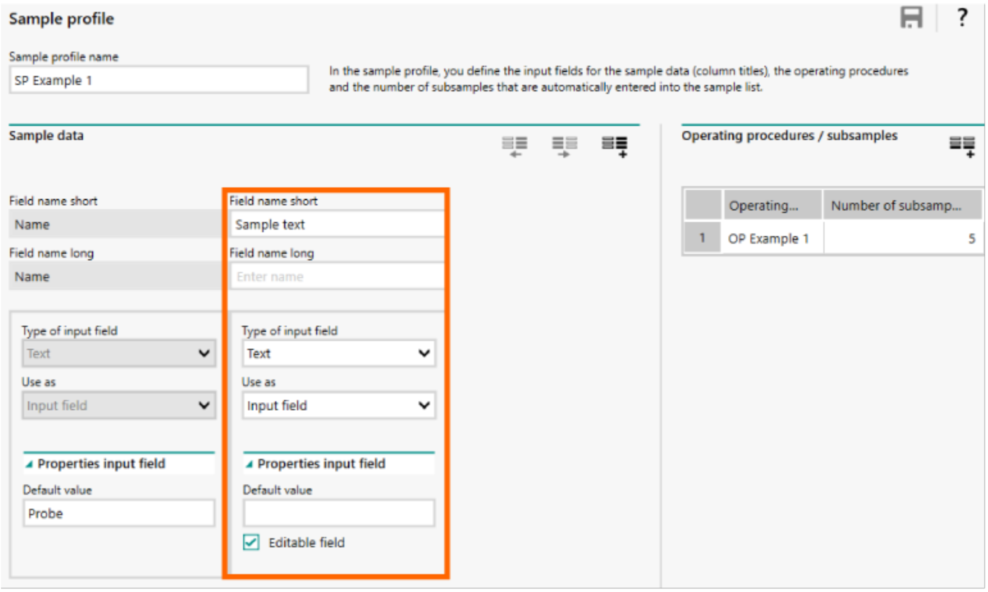
The following characters are not allowed: **.|'"{}**

NOTICE

Further information on creating a sample profile: *Creating and editing a sample profile (see chapter 5.8.4.1, page 176)*

5 Defining sample data

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



- 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 in accordance with the data in the CSV file.
  - The **Editable field** check box is activated.
- 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.

NOTICE

The following characters are not allowed: **.|'"{}**

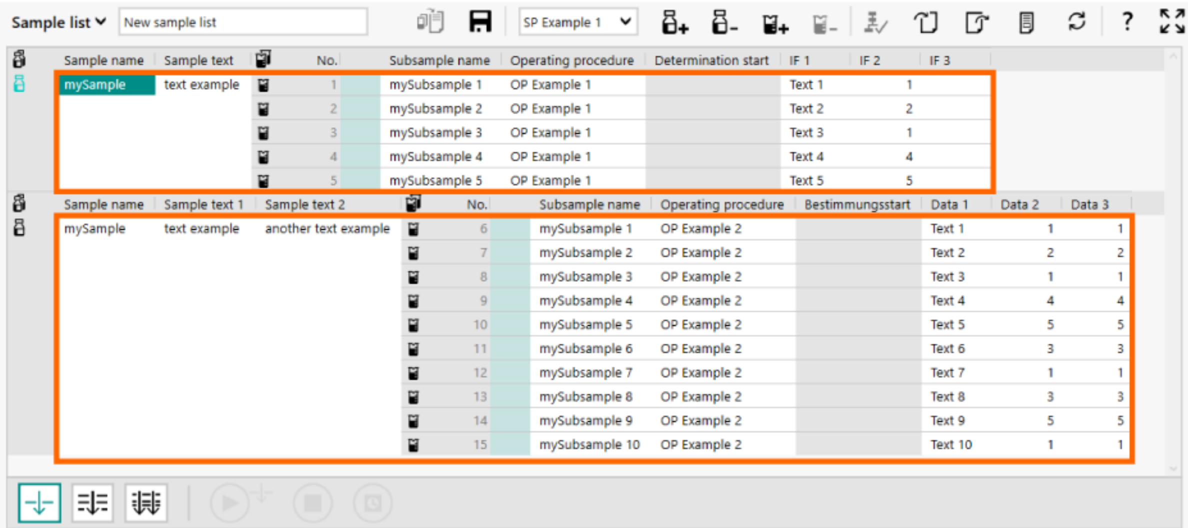
6 Saving the CSV file

- Click on **[Save]** in the table editing program. Select the required memory location.
- Select the **CSV** format as the **File type**. Make sure that the correct separators are used.
- Create the CSV file by clicking on **[Save]**.

NOTICE

In Microsoft Excel, the correct format is called **CSV (Comma Separated Value)**.

If all data is correct, then the CSV file can be imported into the OMNIS Software: *Importing subsample data (see chapter 5.8.5.6, page 197)*



Configuring the decimal separator

NOTICE

These instructions apply for Windows 10.

1 Changing the regional format

- Navigate to the Windows start menu and open the Windows 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**.

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

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Editing subsample data (chapter 5.9.1.8.1, page 275)

5.8.5.6 Importing subsample data

There are 2 options in the OMNIS Software for importing sample data and subsample data:

- *(see "Importing a sample data file (*.osin)", page 197)* containing sample data and subsample data from the OMNIS Software.
- *(see "Importing a CSV file (*.csv)", page 198)* containing sample data and subsample data from a third-party system.

Importing a sample data file (*.osin)

Prerequisite:

- The sample data file (*.osin) is available.
- A sample list is opened and at the front.

1 Import sample data and subsample data

- Click on to open the **Import sample data and subsample data** window in **Samples ► Sample list**.

2 Folder search

- Select the folder in which the import file is saved.

3 Selecting the file type

- Select the *.osin file type at the bottom right of the window.

- Select the import file or enter the name of the import file in the **File name** field.

4 Confirming and importing the selection

- Click on **[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 (*.csv)

Prerequisite:

- The CSV file is prepared according to the instructions: *Preparing a CSV file (see chapter 5.8.5.5, page 189)*.
- 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.

1 Import sample data and subsample data

- Click on to open the **Import sample data and subsample data** window in **Samples ▶ Sample list**.

2 Folder search

- Select the folder in which the import file is saved.

3 Selecting the file type

- Select the *.csv file type at the bottom right of the window.
- Select the import file or enter the name of the import file in the **File name** field.

4 Confirming and importing the selection

- Click on **[Open]** to confirm the selection.

The sample data and subsample data from the file are imported into the opened sample list.

See also

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Editing subsample data (chapter 5.9.1.8.1, page 275)

5.8.6 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

Single determination – Run (chapter 5.8.6.2, page 200)

Series determination – Run (chapter 5.8.6.3, page 201)

Parallel determination – Run (chapter 5.8.6.4, page 202)

Starting a determination (chapter 5.8.6.6, page 207)

Pausing a determination (chapter 5.8.6.8, page 209)

Stopping a determination (chapter 5.8.6.7, page 209)

Subsamples – Statuses (chapter 5.8.5.2, page 184)

5.8.6.1 Run test – Brief description

When a run is started, an automatic run test is carried out. This test checks whether all conditions have been fulfilled for successfully executing an operating procedure. If the run test is successful, the operating procedure is run without a prompt.

The run test can also be triggered manually by clicking . The test's result is shown at the end of the run test.

If the run test finds an error, an error message appears. The run is not carried out. Correct the error before restarting the run test.

NOTICE

The run test can be carried out only if subsamples that have not yet been analyzed are listed in the sample list.

Only the selected subsample is checked in a single determination.

The run test carries out the following points:

Loading the sample data

The sample data entered for a determination is loaded.

Checking the method

- The feasibility of the methods is checked. In the case of non-runnable methods, a prompt will appear asking to carry out the method check and to modify the method accordingly.
- All commands used must have correct parameters.
- A functional unit must be assigned to all instrument-dependent commands.

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.

NOTICE

- Carry out the run test again if you have changed the subsample data.
- Subsamples with invalid data can be saved, but not carried out.
- Number fields must not be empty. Text fields may be empty.

Assigning a determination ID

- A unique determination ID is assigned for each determination.

5.8.6.2 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 run test

The run test checks whether the determination can be run.

If the run test discovers an error, 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 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 5.8.6.1, page 199)

5.8.6.3 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 marking) and can no longer be edited.

The sample list is then run through from top to bottom. For each subsample, the steps **2** - **4** are carried out.

2 – Executing the run test

The run test checks whether the determination can be run.

If the run test discovers an error, 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 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.

> **NOTICE**
>
> If an error occurs during an ongoing series determination, the series determination is stopped. The status of the subsamples that have not yet been analyzed will be reset to **Ready** (light green status marking).

See also

Run test – Brief description (chapter 5.8.6.1, page 199)

5.8.6.4 Parallel determination – Run

> **NOTICE**
>
> 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: *Activating the function license (see chapter 4.2, page 15)*

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 marking) 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. For each subsample, the steps **2** to **4** are carried out.

2 – Executing the run test

At the start of the analysis of each subsample, the run test checks whether the determination can be run.

If the run test finds an error, an error message appears. The error described in the message must be eliminated after the run of the entire parallel determination has been completed. After that, subsamples that contain an error can be reset to the **Ready** status or, alternatively, new subsamples can be created.

NOTICE

If an optional run of the **Execute on error** type is used in the operating procedure, the behavior in case of an error can be defined there.

3 – Reserving functional units

The determination is started once the run test has been successfully performed. 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.

NOTICE

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 activated under **Properties ▶ Execute with** in the operating procedure.
- To release a reserved work system directly after a method has ended, the method has to be selected in the operating procedure and the **Release work system after completing the method** check box must be activated under **Properties ▶ Execute with**.

Additional information on the user-defined reservation behavior: *Configuring a parallel determination (see chapter 5.8.6.5, page 204)*

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.

NOTICE

Frequent errors during parallel determination: *Configuring a parallel determination (see chapter 5.8.6.5, page 204)*

See also

Run test – Brief description (chapter 5.8.6.1, page 199)

Operating procedure – Properties (chapter 5.9.1.2, page 262)

Activating the function license (chapter 4.2, page 15)

Configuring a parallel determination (chapter 5.8.6.5, page 204)

5.8.6.5 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.

NOTICE

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.

NOTICE

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 activated, 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 .

NOTICE

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

- Right-click or left-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 or in the context menu to add the subsample to the running parallel determination.

- **If step 3 was performed:** Click on ▶ to start the parallel determination.

See also

Run test – Brief description (chapter 5.8.6.1, page 199)

Operating procedure – Properties (chapter 5.9.1.2, page 262)

Activating the function license (chapter 4.2, page 15)

Parallel determination – Run (chapter 5.8.6.4, page 202)

5.8.6.6 Starting a determination

NOTICE

Only saved subsamples with the status **Ready** 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: *Subsamples – Statuses (see chapter 5.8.5.2, page 184)*

1 Selecting determination types

- **Single determination**:

  Click on the button below the sample list.
- **Series determination**:

  Click on the button below the sample list.
- **Parallel determination**:

  Click on the button below the sample list.

2 Selecting the subsample

- Select the desired subsample or subsamples in the sample list.

3 Starting a determination

- Click on ▶.

NOTICE

If the work system required for a determination is occupied, the determination will not be started until the work system is once again free.

- **Single determination**:
  The operating procedure for the determination of the selected subsample is started. No additional subsample can be added for analysis during a single determination.
- **Series determination**:
  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.
- **Parallel determination**:
  The parallel determination starts with the first executable subsample. This subsample receives the focus and is highlighted in dark green. All executable subsamples from the sample list are then analyzed in sequence. Up to four subsamples can be in the **Running** status at the same time. The focus switches automatically thereby to the next subsample currently being executed.

NOTICE

If an operating procedure present in the sample list is changed in **Processes ▶ Operating procedures** but has not yet been started, 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. These subsamples are reset again to **Ready**. To accomplish this, click on the respective subsample to open the context menu and select **Remove from running sample series**.

See also

Stopping a determination (chapter 5.8.6.7, page 209)

Subsamples – Statuses (chapter 5.8.5.2, page 184)

5.8.6.7 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 a determination (chapter 5.8.6.6, page 207)

Subsamples – Statuses (chapter 5.8.5.2, page 184)

5.8.6.8 Pausing a determination

The **Hold determination** function is used to pause the running operating procedure.

NOTICE

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.

1 Pausing a sequence

- In the sample list, click on the status of the subsample to call up the context menu and select **Hold determination**r.

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
- Calibration commands
- Dosing commands such as**ADD**, **PISTON END** or **FILL**
- Time-controlled commands: **PUMP**, **STIR**, **WAIT** or **READ**
- Additional commands: **REQUEST**

NOTICE

For dosing commands, the execution is paused when the Hold determination function is selected. Clicking on **Continue** causes the command is be resumed at the position where it was paused.

For time-controlled commands, the time 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 such as**LIFT**, **OPEN GRIPPER** or **CLOSE GRIPPER**
- Additional commands e.g.**WRITE**, **TARE** or **WEIGH**

See also

Subsamples – Statuses (chapter 5.8.5.2, page 184)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

COND CHECK – Parameters (chapter 5.9.4.2.14.1, page 442)

5.8.6.9 Preparing the determination

These instructions summarize all the individual steps necessary for performing determinations in the OMNIS Software. Links to specific topics are included for more information on individual steps.

Preparing the sample

Prerequisite:

- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Reserving an instrument and creating a work system

- Reserve the desired instruments in **Equipment ▶ Instruments**. *Reserving instruments (see chapter 5.10.1.3, page 666)*
- In **Equipment ▶ Work systems**, click on **+** to create a new work system. *Creating a work system (see chapter 5.10.3.2, page 785)*
- 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 a method

- In **Processes ▶ Methods**, click on **+** to create a new method.*Creating and editing a method (see chapter 5.9.2.3, page 284)*
- In the new method, click on to open the **Properties** window.

- In **Properties ▶ Execute with**, select the work system created in **step 1**.

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**. *Assigning functional units to a command (see chapter 5.10.2.3, page 706)*
- If required, insert an optional run. *Creating and editing a method (see chapter 5.9.2.3, page 284)*
- Save the method by clicking on .

4 Creating an operating procedure

- In **Processes ▶ Operating procedure**, click on to create a new operating procedure. *Creating and editing an operating procedure (see chapter 5.9.1.3, page 265)*
- Click on to open the **Library** window and use drag and drop in **Library ▶ Methods** to insert the method created in **step 2** in the operating procedure.
- If required, insert further methods into the operating procedure.
- Click on to save the operating procedure.

5 Creating a sample profile

- Create a new sample profile under **Samples ▶ Sample profiles** by clicking on . *Creating and editing a sample profile (see chapter 5.8.4.1, page 176)*
- Assign an unambiguous name for the sample profile in the **Sample profile name** field. This name is needed to identify the sample profile (see **step 6**) when creating the sample.
- Select the operating procedure created in **step 4** and define the required number of subsamples.
- Save the sample profile by clicking on .

6 Creating and editing a sample list

- Under **Samples ▶ Sample lists**, click on to create a new sample list. *Creating and deleting a sample list (see chapter 5.8.1.1, page 142)*

- In the sample list, select the sample profile created in **step 5** and add the required number of samples to the sample list by clicking on **+**. The samples and associated subsamples are inserted in the sample list automatically in accordance with the sample profile.
- Save the sample list by clicking on .

7 Carrying out the determination

- **Optional**: To process all samples one after the other, set the determination as a series determination by clicking on .
- Start the determination by clicking on . *Starting a determination (see chapter 5.8.6.6, page 207)*

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Reserving instruments (chapter 5.10.1.3, page 666)

Creating a work system (chapter 5.10.3.2, page 785)

Creating and editing a method (chapter 5.9.2.3, page 284)

Assigning functional units to a command (chapter 5.10.2.3, page 706)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Creating and editing a sample profile (chapter 5.8.4.1, page 176)

Sample list – Tab (chapter 5.2.3, page 100)

Starting a determination (chapter 5.8.6.6, page 207)

5.8.6.10 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.

NOTICE

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.

NOTICE

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.

> **NOTICE**
>
> The variables must be inserted again in the formula editor if a method is renamed for which variables are used in the **IF** command.

> **NOTICE**
>
> 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

Variables – Directory (chapter 5.9.5.3, page 640)

IF – Parameters (chapter 5.9.4.16.5, page 595)

Work system – Definition (chapter 5.10.3, page 783)

5.8.7 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**.

NOTICE

Requirement for all instructions:

The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

Requirement for working with prediction models:

The license to edit prediction models is available.

Displaying the 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 the 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.

NOTICE

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.

NOTICE

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. Further information for the **Properties** window: *Curves – Properties (see chapter 5.8.10, page 225)*

Hiding and showing the measured value window or details window

Prerequisite:

- The **Samples ▶ Sample lists** or **Samples ▶ Search queries** subsection is opened.
- One of the following areas is visible:
  - **Calibration curves**
  - **Curves**
  - **Live data**
- The **Models ▶ Prediction 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

NOTICE

The following instructions apply for all charts in the work areas **Samples** and **Models**.

1 Copying the chart or the table

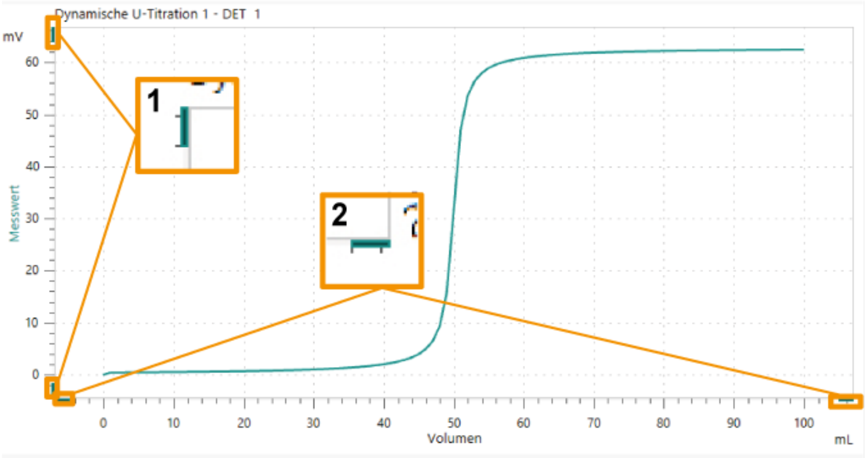
- Right-click in the chart or table.
- Select **[Copy chart]** in the context menu.
  or
- Select **[Copy table]** in the context menu.

The chart or table is copied to the clipboard.

2 Inserting the chart or table

- Open the required document in which the chart or table is to be inserted.
- Insert the chart or the table into the document.

Scaling the 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 the 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 the 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 the keyboard and the cursor

1 Positioning the cursor

- Position the cursor on the desired section in the graphics window.

2 Zooming the chart vertically

- Rotate the mouse wheel while holding the **[CTRL]** key pressed down.
  - Rotate forward: Increase section vertically.
  - Rotate backward: Decrease section vertically.

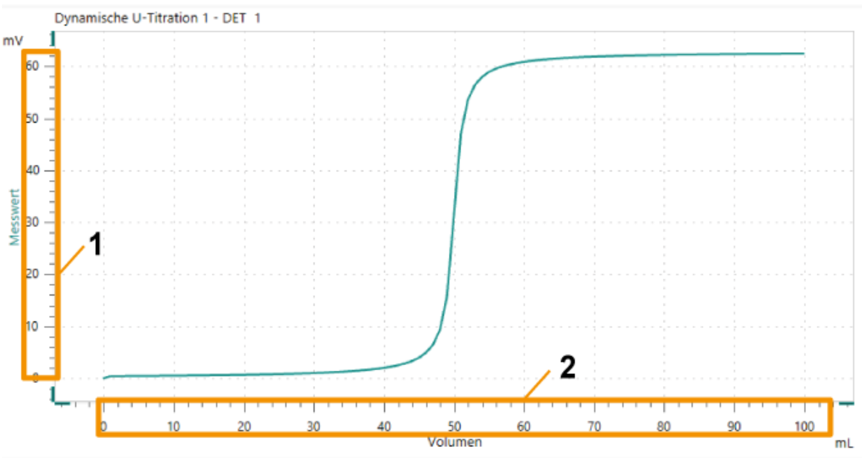
3 Zooming the chart horizontally

- Rotate the mouse wheel while holding the **[SHIFT]** key pressed down.
  - Rotate forward: Increase section horizontally.
  - Rotate backward: Decrease section horizontally.

4 Scaling the x-axis and y-axis together

- Rotate the mouse wheel.
  - Rotate forward: Increase section horizontally and vertically.
  - Rotate backward: Decrease section horizontally and vertically.

Moving the displayed area



1 Moving the 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 the 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 the display

1 Resetting the 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 left to right.

The chart is reset to the default view.

See also

Curves – Properties (chapter 5.8.10, page 225)

Reevaluating curves (chapter 5.8.17, page 240)

Displaying live data and controlling run (chapter 5.8.9, page 222)

Displaying a measuring point list (chapter 5.8.8, page 221)

5.8.8 Displaying a measuring point list

Prerequisites:

- 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 measuring point list is to be displayed.

2 Displaying a measuring point list

- In **Curves and data ▶ Measuring point lists**, display the measuring points that were recorded during the determination for the selected subsample.

NOTICE

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.

Copying a table

The table with the measuring point list is to be used outside of the software.

1 Copying a table

- Right-click on the table.
- Select **[Copy table]** in the context menu.

The table is copied to the clipboard.

2 Inserting a table

- Open the required document in which the table is to be inserted.
- Insert the table in the document.

See also

Sample list – Tab (chapter 5.2.3, page 100)

5.8.9 Displaying live data and controlling 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

Prerequisites:

- 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.

NOTICE

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.

NOTICE

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	Indication
	The drift decreases.
	The drift increases.
	The drift is stable.

NOTICE

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]**.

NOTICE

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 grayed out.

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 next command.

Ending conditioning prematurely and starting the 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.

NOTICE

The titration is started from the **Conditioning not OK** status.

- Click on **[Continue conditioning]** to return to conditioning.

See also

Sample list – Tab (chapter 5.2.3, page 100)

Displaying curves and adjusting the curve display (chapter 5.8.7, page 216)

5.8.10 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).

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).

See also

Displaying curves and adjusting the curve display (chapter 5.8.7, page 216)

Reevaluating curves (chapter 5.8.17, page 240)

Overlaying curves (chapter 5.8.16, page 238)

DET – Properties (chapter 5.9.4.2.1.2, page 299)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

CAL CONC – Properties (chapter 5.9.4.13.2, page 513)

CAL COND – Properties (chapter 5.9.4.13.3, page 521)

CAL pH – Properties (chapter 5.9.4.13.1, page 504)

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

MEAS Ipol – Properties (chapter 5.9.4.12.4.1, page 484)

MEAS pH – Properties (chapter 5.9.4.12.2.1, page 472)

MEAS T – Properties (chapter 5.9.4.12.5, page 490)

MEAS U – Properties (chapter 5.9.4.12.3.1, page 478)

5.8.11 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:

NOTICE

In the case of equivalence point titrations, the functions and parameters for the automatic evaluation in the **Reevaluation** window are displayed only if the **[Automatic]** option is selected in the window. If equivalence points have been added or deleted previously in the manual evaluation, these changes are 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: *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*.
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: *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*

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: *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*.
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. *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*

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: *Curves – Gran evaluation (see chapter 5.8.15, page 235)*

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

Reevaluating curves (chapter 5.8.17, page 240)

Curves – Manual evaluation (chapter 5.8.14, page 234)

Curves – Fixed point evaluation (chapter 5.8.13, page 233)

Curves – Gran evaluation (chapter 5.8.15, page 235)

DET – Properties (chapter 5.9.4.2.1.2, page 299)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

5.8.12 Curves – Window-based evaluation

The window definitions can be individually added by clicking on or deleted by clicking on .

NOTICE

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

The Potentiometric evaluation can be carried out with or without window evaluation.

For the potentiometric 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 or Potential 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.
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.
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 – Manual evaluation (chapter 5.8.14, page 234)

DET – Properties (chapter 5.9.4.2.1.2, page 299)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

Curves – Automatic evaluation (chapter 5.8.11, page 226)

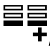
Reevaluating curves (chapter 5.8.17, page 240)

5.8.13 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. A fixed point can be defined using one of the following three measured quantities:

- Measured value (pH value or potential)
- Volume
- Point in 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 that is recognized as 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 5.9.4.2.1.2, page 299)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

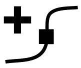
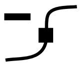
5.8.14 Curves – Manual evaluation

Clicking under **Samples ▶ Sample list ▶ Subsample ▶ Curves and data ▶ Curves** opens the **Reevaluation** window. The following functions are available for equivalence point titrations when **[Manual]** is selected:

NOTICE

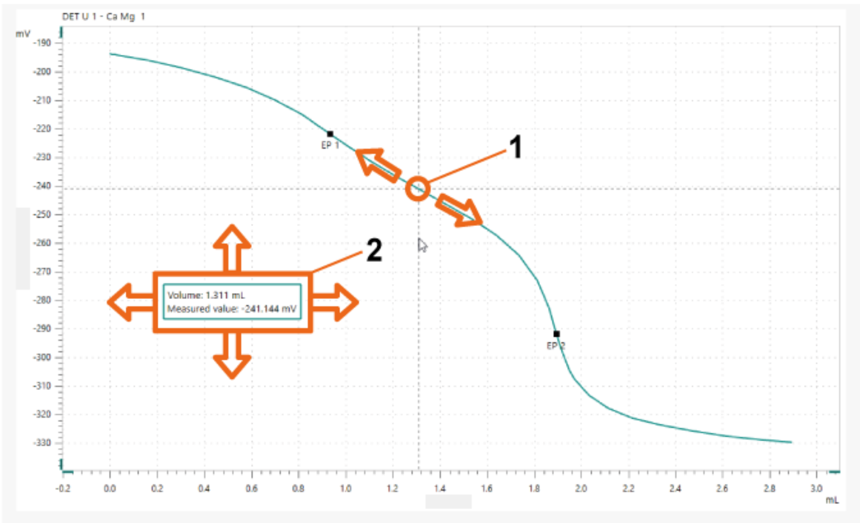
To edit equivalence points (EPs) manually, at least one of the following quantities must be selected for the x-axis or y-axis in the Properties of the curve:

- Volume
- Time

	**[Add EP]** Click the curve to add an additional equivalence point. The equivalence points are renumbered automatically. The crosshair is displayed as an aid to positioning the equivalence point on the curve (see *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 moved 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 holding.

See also

Curves – Properties (chapter 5.8.10, page 225)

Displaying curves and adjusting the curve display (chapter 5.8.7, page 216)

Reevaluating curves (chapter 5.8.17, page 240)

Curves – Automatic evaluation (chapter 5.8.11, page 226)

5.8.15 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 is used for linearization of the measuring points. This depends on two factors:

- Reaction type (analyte, titrant)
- Evaluation ranges of the titration curve (segment before the equivalence point, segment after the equivalence point or both segments)

The Gran function and the range used for the determination of the Gran point 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 displayed as a result in the Gran plot 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 area of the segment which 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.

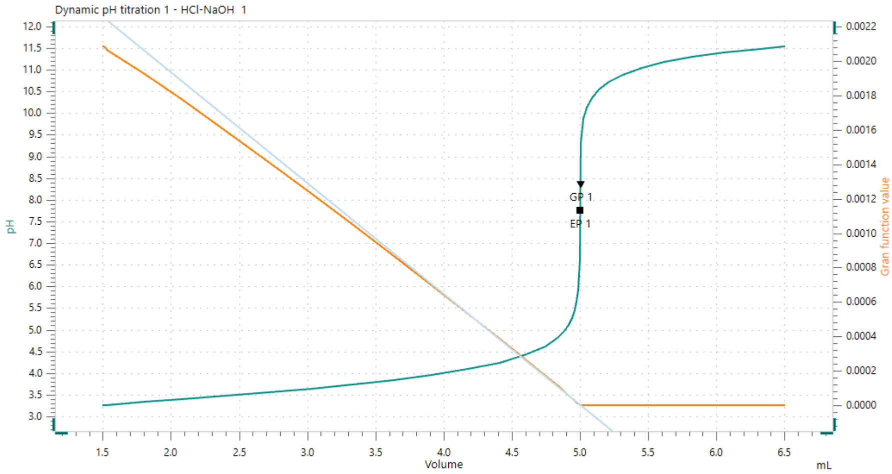
The following Gran functions are used for acid-base titrations in accordance with Gunnar Gran (1952. Determination of the Equivalence Point in Potentiometric Titrations. Part II. The Analyst, 77, 661-671):

Reaction type	Segment	Gran function
Weak monoprotic acid, strong base	Acidic segment before the equivalence point	$G_{before}\big(V(t), pH(t)\big) = V(t) \cdot 10^{(k - pH(t))}$
	Alkaline segment after the equivalence point	$G_{after}\big(V(t), pH(t)\big) = \big(V_0 + V(t)\big) \cdot 10^{(pH(t) - k)}$
Weak monoprotic base, strong acid	Alkaline segment before the equivalence point	$G_{before}\big(V(t), pH(t)\big) = V(t) \cdot 10^{(pH(t) - k)}$
	Acidic segment after the equivalence point	$G_{after}\big(V(t), pH(t)\big) = \big(V_0 + V(t)\big) \cdot 10^{(k - pH(t))}$
Strong acid, strong base	Acidic segment before the equivalence point	$G_{before}\big(V(t), pH(t)\big) = \big(V_0 + V(t)\big) \cdot 10^{(k - pH(t))}$
	Alkaline segment after the equivalence point	$G_{after}\big(V(t), pH(t)\big) = \big(V_0 + V(t)\big) \cdot 10^{(pH(t) - k)}$
Strong base, strong acid	Alkaline segment before the equivalence point	$G_{before}\big(V(t), pH(t)\big) = \big(V_0 + V(t)\big) \cdot 10^{(pH(t) - k)}$
	Acidic segment after the equivalence point	$G_{after}\big(V(t), pH(t)\big) = \big(V_0 + V(t)\big) \cdot 10^{(k - pH(t))}$

Example of a Gran evaluation in 1 segment

Reaction type	Strong acid, strong base
Gran plot	Acidic segment

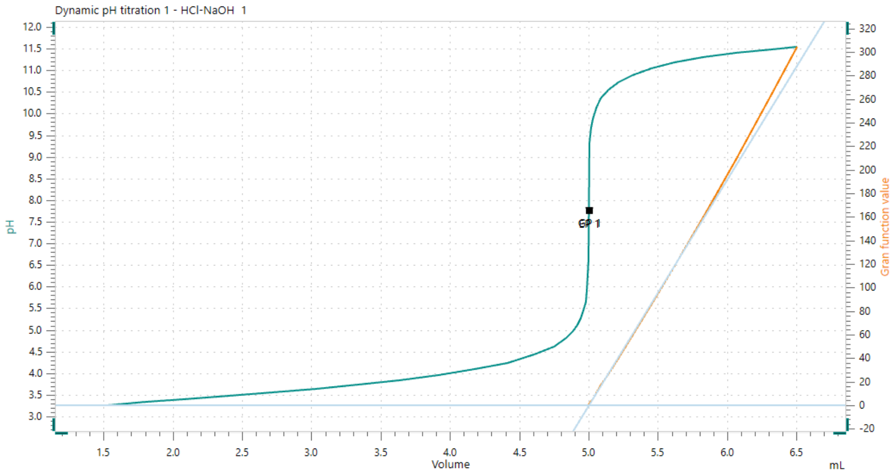
In the curve display, the curve is presented from the Gran function values, the regression line and the Gran point (GP).



Example of a Gran evaluation in 2 segments

Reaction type	Strong acid, strong base
Gran plot	Acidic and alkaline segment

In the curve display, the curve is presented from the Gran function values, the regression line and the Gran point (GP).



See also

DET – Run (chapter 5.9.4.2.1.3, page 317)

DET – Properties (chapter 5.9.4.2.1.2, page 299)

MET – Run (chapter 5.9.4.2.2.3, page 341)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

5.8.16 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.

NOTICE

In order for all curves to be displayed, the curves must have the same quantities for the x-axis and y-axis.

1 Selecting the 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.

NOTICE

Additional information about selecting several subsamples: *Editing a sample list (see chapter 5.8.1.2, page 143)*

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 settings.

NOTICE

Additional subsamples can be selected if necessary to add their curves to the curve overlay.

NOTICE

If the icon is not displayed, the area has to be enlarged by dragging the separating bar.

Actions in the overview list

1 Sorting curves

- Sort the displayed curves by clicking on the required column title in the overview list.

2 Hiding and showing curves

- Hide a curve by deactivating the check box in the first column of the overview list.

NOTICE

The curve is shown again if you activate the check box.

In case not all curves are displayed

1. Click on to deactivate the curve overlay.
2. Select an affected subsample in the sample list.
3. Click on to open the **Properties** window.
4. For the x-axis, y-axis or y2-axis, compare the selected quantity in the **Quantity** input field with the measured quantities of the curves that are not being displayed and, if necessary, adjust the information.
5. Repeat the procedure for each affected subsample.

See also

Reevaluating curves (chapter 5.8.17, page 240)

Curves – Properties (chapter 5.8.10, page 225)

Displaying curves and adjusting the curve display (chapter 5.8.7, page 216)

5.8.17 Reevaluating curves

Prerequisite:

- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*
  The **Samples ▶ Sample lists** subsection is opened. A sample list is opened and at the front.

1 Selecting the 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**.

> **NOTICE**
>
> 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 Select the type of reevaluation (only for equivalence point titrations)

- 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 at the time of the automatic evaluation: *Curves – Automatic evaluation (see chapter 5.8.11, page 226)*
  or

- Adding, editing or removing equivalence points at the time of the manual evaluation: *Curves – Manual evaluation (see chapter 5.8.14, page 234)*

NOTICE

As soon as the field in which the changes have been made is exited, the curve is reevaluated with the modified parameters. 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 5.8.10, page 225)

Displaying curves and adjusting the curve display (chapter 5.8.7, page 216)

5.8.18 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.

NOTICE

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.

Copying a table

The table with the raw data, calculations, statistics or monitoring is to be used outside of the software.

1 Copying a table

- Right-click on the table.
- Select **[Copy table]** in the context menu.

The table is copied to the clipboard.

2 Inserting a table

- Open the required document in which the table is to be inserted.
- Insert the table in the document.

See also

Reprocessing calculations (chapter 5.8.19.1, page 244)

Reprocessing Sample statistics (chapter 5.8.20, page 247)

5.8.19 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.

> **NOTICE**
>
> 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 **PropertiesParameters**.
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**.

NOTICE

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

Reprocessing calculations (chapter 5.8.19.1, page 244)

Reprocessing Sample statistics (chapter 5.8.20, page 247)

Filtering Search queries (chapter 5.8.2.3, page 167)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

5.8.19.1 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**.

NOTICE

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 fx= to open the **Calculation parameters** window.
- Edit the calculation parameters as desired.

NOTICE

More information on the parameters: *CALC – Parameters (see chapter 5.9.4.16.1, page 586)*

The parameters **Result unit**, **Decimal places** and **Formula** can be recalculated.

The subsample with the reprocessed calculations is marked with .

NOTICE

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 .

NOTICE

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**.

NOTICE

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

Displaying the results (chapter 5.8.18, page 241)

User rights – Directory (chapter 4.6.7.3, page 62)

CALC – Parameters (chapter 5.9.4.16.1, page 586)

Reprocessing subsample data (chapter 5.8.5.4, page 188)

Reprocessing Sample statistics (chapter 5.8.20, page 247)

5.8.20 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.

NOTICE

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.

NOTICE

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 subsample data (chapter 5.8.5.4, page 188)

Reprocessing calculations (chapter 5.8.19.1, page 244)

5.8.21 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.

NOTICE

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.

NOTICE

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.

NOTICE

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 5.9.1.3, page 265)

Recording subsamples (chapter 5.8.5.1, page 181)

Subsamples – Statuses (chapter 5.8.5.2, page 184)

Reprocessing calculations (chapter 5.8.19.1, page 244)

Creating and editing a sample profile (chapter 5.8.4.1, page 176)

5.8.22 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

Result monitoring – Definition (chapter 5.9.1.9, page 278)

Filtering Search queries (chapter 5.8.2.3, page 167)

Filtering the monitoring status (chapter 5.8.22.2, page 253)

5.8.22.1 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 **SamplesSample listResultsMonitoring** with their status icons.

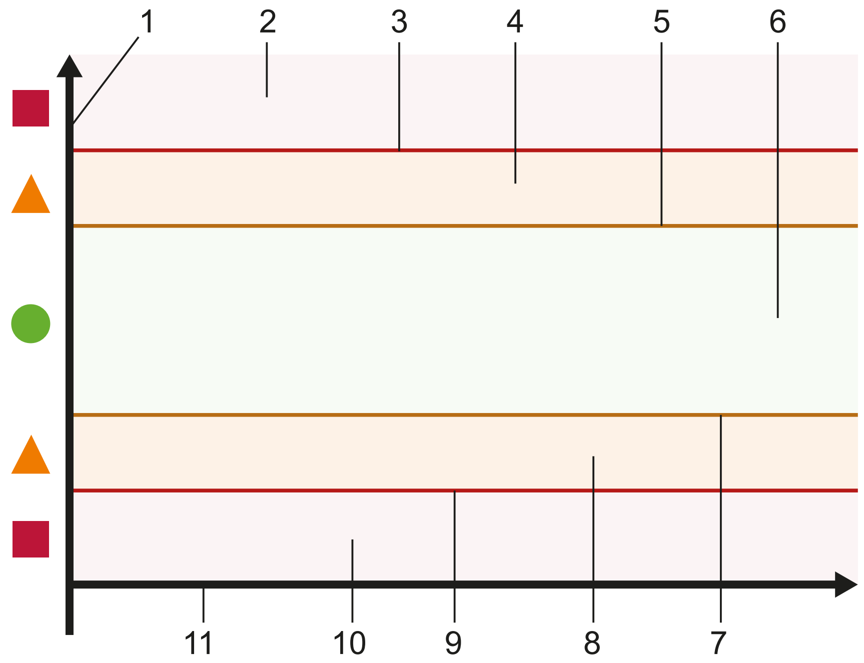
Depending on the defined limits, monitored results are displayed with the following status icons:

	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**.

NOTICE

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

Activating sensor monitoring (chapter 5.10.5.9, page 813)

Sensor – Properties (chapter 5.10.5.2, page 798)

5.8.22.2 Filtering the monitoring status

NOTICE

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).

NOTICE

To reset the filter or to delete or save it, perform steps 7 - 10 *Filtering Search queries (see chapter 5.8.2.3, page 167)*.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Sample list – Tab (chapter 5.2.3, page 100)

Recording the result monitoring (chapter 5.9.1.9.1, page 278)

Result monitoring – Status (chapter 5.8.22.1, page 251)

Search queries – Definition (chapter 5.8.2, page 165)

Creating a Search queries (chapter 5.8.2.2, page 166)

Monitoring – Definition (chapter 5.8.22, page 251)

5.8.23 Predictions – Subsection

In **Sample list ▶ Results ▶ Predictions**, the predictions are displayed in a table which was created by the **PREDICT** commands for selected subsamples. If the prediction model and the slope/y-intercept correction in the **PREDICT** command correspond (name and version), the predictions from various subsamples are grouped and displayed in one table.

Table

The following information about the selected subsample is shown in the table of the corresponding prediction model:

Subsample name	Name of the subsample.
Calculated value	Value that was determined by using the prediction model on the selected spectrum without the use of a slope/y-intercept correction.
Corrected value	Value that was determined by using the prediction model on the selected spectrum with the use of a slope/y-intercept correction. If no slope/y-intercept correction was used, this value is identical to the calculated value.

After selecting a prediction model in the **Repredict with** field or a slope/y-intercept correction in the **Correct with** field, the following information is displayed in the table:

Subsample name	Name of the subsample.
Old value	Numerical value of the original prediction. If a slope/y-intercept correction was used, the corrected value is entered.
New value	Numerical value of the repredicted prediction. If a slope/y-intercept correction was used, the corrected value is entered.
Repredicted with	Name of the prediction 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, **No correction** is entered.

Additional details on the used prediction model or the slope/y-intercept correction are displayed in the table under **Detail view**.

See also

PREDICT – Parameters (chapter 5.9.4.3, page 447)

Reevaluating the prediction (chapter 5.8.23.1, page 256)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Slope/y-intercept correction – Definition (chapter 5.11.2.7, page 915)

5.8.23.1 Reevaluating the prediction

In **Samples ▶ Results ▶ Predictions**, the results are displayed that were created by the **PREDICT** command for the selected subsamples.

Prerequisite:

- The **Samples ▶ Sample lists** subsection is opened.
- The **Results ▶ Predictions** subsection is opened in the open sample list.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Selecting subsamples

- Select the subsamples in the sample list that are to be repredicted.

NOTICE

Additional information on the multiple selection in the sample list: *Editing a sample list (see chapter 5.8.1.2, page 143)*

In the **Results ▶ Predictions** subsection, the calculated values and result values of the selected subsamples are displayed.

2 Repredicting results

- In the **Results ▶ Predictions** subsection in the **Repredict with** field, select the prediction model with which the results are to be repredicted.
  or
- In the **Results ▶ Predictions** subsection in the **Correct with** field, select the slope/y-intercept correction with which the results are to be corrected.
  or
- Fill in both of the above fields, if both a reprediction and a correction are to be carried out.

A table with the following details is displayed: Subsample name, Old value, New value, Repredicted with, Corrected with.

The subsamples with repredicted predictions are marked with .

3 Saving the sample list

- Save the sample list by clicking on .

The subsamples are marked with .

See also

User rights – Directory (chapter 4.6.7.3, page 62)

CALC – Parameters (chapter 5.9.4.16.1, page 586)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Editing a Prediction model (chapter 5.11.1.5, page 875)

Publishing a prediction model (chapter 5.11.1.17, page 903)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Displaying the results (chapter 5.8.18, page 241)

5.8.24 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 5.8.24.1, page 258)

Samples – Actions (chapter 5.8, page 140)

Sorting the overview list (chapter 5.2.10, page 117)

5.8.24.1 Creating system variables

Creating system variables

1 Setting up a system variable

- Click on (x)+ in **Samples ▶ System variables**.
- Alternatively, open the context menu by right-clicking on a line and select the **[Create system variable]** function.

A new line is created.

2 Naming a system variable

- Enter the desired name in the name field for the new system variable and confirm with **[Enter]**.

NOTICE

Each name can only be given 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 a system variable

- Save the system variable by clicking on .

The date and the time the system variables were saved are displayed in the **Saved** field.

Deleting a system variable

The system variable must have been saved.

1 Selecting a system variable

- Mark the line by clicking on the numbering. Open the context menu by right-clicking on the highlighted cell and select the **[Delete]** function.

2 Confirming the message

NOTICE

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 until that variable is recreated as system variable with the original name or until it is replaced by another variable.

- Click on **[OK]** to confirm the action.
- Alternatively cancel the action by clicking on **[Cancel]**.

The system variable is deleted.

See also

Samples – Definition (chapter 5.8.3, page 171)

System variables – Definition (chapter 5.8.24, page 257)

Sorting the overview list (chapter 5.2.10, page 117)

5.9 Processes – Actions

You can execute the following actions 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**.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Operating procedure – Definition (chapter 5.9.1, page 260)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Method – Definition (chapter 5.9.2, page 281)

Creating and editing a method (chapter 5.9.2.3, page 284)

Tags – Definition (chapter 5.7, page 137)

Creating and editing tags (chapter 5.7.1, page 137)

Creating a signature (chapter 5.6.1, page 132)

Deleting a signature (chapter 5.6.3, page 135)

Audit trail work area – Actions (chapter 5.12, page 917)

5.9.1 Operating procedure – Definition

An **operating procedure** defines the work sequence for the analysis of subsamples. This work run is defined using **methods** and device-independent **commands** that can be aligned sequentially and in parallel.

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.

See also

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Method – Definition (chapter 5.9.2, page 281)

Command – Properties (chapter 5.9.4.1, page 295)

Subsample data – Definition (chapter 5.9.1.8, page 274)

User rights – Directory (chapter 4.6.7.3, page 62)

Report template – Directory (chapter 5.8.1.4, page 155)

Creating and editing tags (chapter 5.7.1, page 137)

Filtering operating procedures and methods (chapter 5.9.1.4, page 270)

Creating a signature (chapter 5.6.1, page 132)

Deleting a signature (chapter 5.6.3, page 135)

Audit trail work area – Actions (chapter 5.12, page 917)

5.9.1.1 Operating procedures – Subsection

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 operating procedures. If the import files contain OMNIS methods and work systems, then these can also be imported.
- Use **Export operating procedures** to export the operating procedure with all contained methods as a file. The work systems used in the method can be added to the export file.
- Use **Create parameter report** to create a parameter report for the selected operating procedure.
- Use **Duplicate operating procedure** to duplicate the selected operating procedure under the same name. The new operating procedure contains the same methods, commands and parameters as the original operating procedure.
- The properties of the selected element are displayed in the **Properties** window.
- Use **Delete operating procedure** to delete the operating procedure. Methods contained in the operating procedure are retained in the database.

NOTICE

Operating procedures can be filtered by names and tags.

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.
Saved	Time at which the sample list was last saved.
Version	Version number of the object. A new version is created automatically each time the object is saved.
Tags	Existing tags assigned to this operating procedure.

See also

Operating procedure – Definition (chapter 5.9.1, page 260)

Operating procedure – Properties (chapter 5.9.1.2, page 262)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Exporting operating procedure and method (chapter 5.9.1.6, page 272)

Filtering operating procedures and methods (chapter 5.9.1.4, page 270)

Importing operating procedure and method (chapter 5.9.1.5, page 271)

Operating procedure and method – Tab (chapter 5.2.6, page 108)

5.9.1.2 Operating procedure – Properties

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 6 subsections **General**, **Parameters**, **Execute with**, **Result monitoring**, **Reports** and **Export**:

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 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, if this method is contained several times in an operating procedure.

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 **Operating procedure** is selected, the **Work systems reservation behavior** section is displayed. The following functions are available:

Reserve work systems only when needed	If this check box is enabled, work systems can be selected that are to be reserved 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: *Configuring a parallel determination (see chapter 5.8.6.5, page 204)*

If a **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: *Configuring a parallel determination (see chapter 5.8.6.5, page 204)*
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 activated, this setting applies for all run sequences of this type within the separate methods, but also within the entire operating procedure.

If a **Command** within a method is selected, then the functional units assigned to the command are displayed.

Result monitoring

Clicking on the **[Monitor results]** button allows result monitoring to be defined and edited. Additional information on the result monitoring:*Recording the result monitoring (see chapter 5.9.1.9.1, page 278)*

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 creating reports: *Creating a report (see chapter 5.8.1.5, page 159)*

> **NOTICE**
>
> 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: *REPORT – Parameters (see chapter 5.9.4.16.11, page 607)*

Export

An export can be generated automatically after the completion of a determination. A new export can be defined by clicking on . can be used to delete an export definition once again. Additional information on exporting: *Exporting subsample data (see chapter 5.8.1.3, page 151)*

> **NOTICE**
>
> 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.

See also

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Setting up a printer (chapter 5.13.1, page 932)

EXPORT – Parameters (chapter 5.9.4.16.4, page 593)

Formula editor – Brief description (chapter 5.9.5, page 637)

Method – Properties (chapter 5.9.2.2, page 283)

Parallel determination – Run (chapter 5.8.6.4, page 202)

REPORT – Parameters (chapter 5.9.4.16.11, page 607)

Result monitoring – Definition (chapter 5.9.1.9, page 278)

Editing subsample data (chapter 5.9.1.8.1, page 275)

5.9.1.3 Creating and editing an operating procedure

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**.

NOTICE

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 **Properties ▶ General** in the **Name** field.

NOTICE

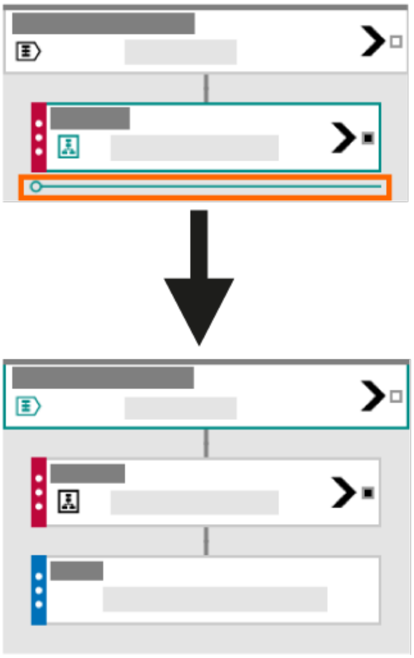
The following characters are not allowed: **.|'"{}**

3 Inserting methods and commands

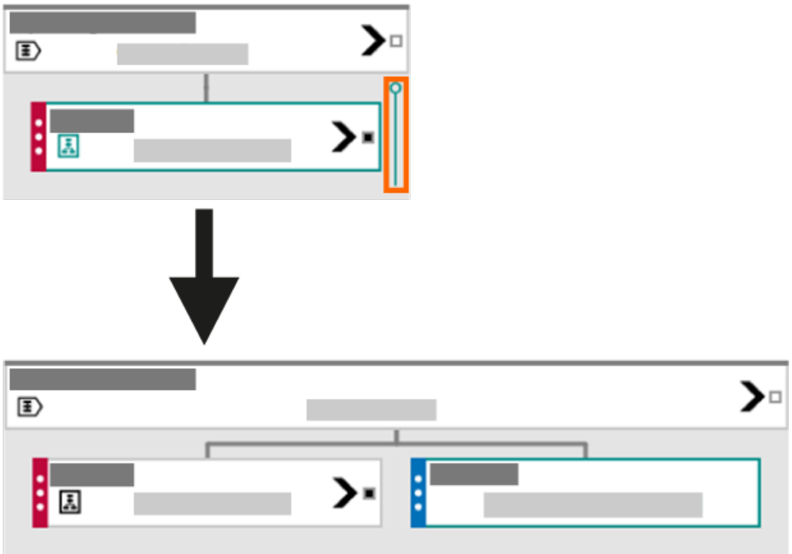
- Click on to open the **Library** window.
- Use drag and drop to insert the desired methods into the operating procedure in **Library ▶ Methods**.
- Use drag and drop to insert the desired commands into the operating procedure in **Library ▶ Commands**.

The methods and commands can be inserted either one below the other or side by side:

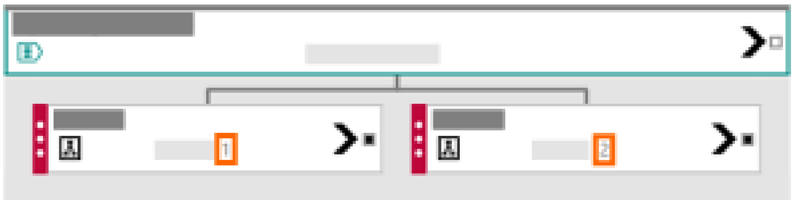
- Commands and methods that are aligned one below the other are executed **sequentially**. A green horizontal line shows the insertion position of an object.



- 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.



NOTICE

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.

4 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.

NOTICE

An optional sequence can be inserted only parallel to the run. Further information on the optional runs:

Run in case of a stop – Definition (see chapter 5.9.3.2, page 292)

Run in case of an error – Definition (see chapter 5.9.3.1, page 291)

Run in case of a limit value violation – Definition (see chapter 5.9.3.3, page 293)

5 Editing command parameters

- Select the desired command.
- Click on to open the **Properties** window.
- Change the desired command parameter in **Properties ▶ Parameters**.

6 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.

7 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 *Recording the result monitoring (see chapter 5.9.1.9.1, page 278)*.

8 Defining reports

- Click on 

.
- Click on to open the **Properties** window.
- Select the **Properties ▶ Reports** subsection.

- Define the reports according to the instructions in *Creating a report (see chapter 5.8.1.5, page 159)*.

9 Defining exports

- Click on Operating Procedure.
- Click on to open the **Properties** window.
- Select the **Properties ▶ Exports** subsection.
- Define the exports according to the instructions in *Exporting subsample data (see chapter 5.8.1.3, page 151)*.

10 Saving the operating procedure

- Click on to save the operating procedure.

The operating procedure is saved. The version and change date of the operating procedure are updated automatically in the **Properties ▶ General** subsection.

See also

Creating and editing a method (chapter 5.9.2.3, page 284)

Editing subsample data (chapter 5.9.1.8.1, page 275)

5.9.1.4 Filtering operating procedures and methods

1 Selecting the overview list

- Open the **Processes ▶ Operating procedures** area if filtering is to be performed according to operating procedures.
  or
- Open the **Processes ▶ Methods** area if filtering is to be performed according to methods.

2 Filtering by names (optional)

- Enter the name of the operating procedure or method you are searching for in the **[Enter name]** input field.

Only the operating procedures / methods that contain the entered term in their name are listed.

3 Filtering by tags (optional)

- In the **[Enter tags]** input field, enter the name of a tag that is assigned to the operating procedures / methods you are looking for.

Only operating procedures / methods that were assigned the entered tag are listed.

NOTICE

Names and tags can be combined to limit the search results further.

See also

Tags – Definition (chapter 5.7, page 137)

Creating and editing tags (chapter 5.7.1, page 137)

Operating procedure – Definition (chapter 5.9.1, page 260)

Method – Definition (chapter 5.9.2, page 281)

5.9.1.5 Importing operating procedure and method

1 Selecting an operating procedure or method

- Click on to open the **Import method / operating procedure** window in **Processes ▶ Operating procedures**.
  or
- Click on to open the **Import method / operating procedure** window in **Processes ▶ Methods**.

2 Browsing for folder

- Select the folder in which the import file is saved.

3 Selecting the file type

- Select the *.opro file type at the bottom right of the window.
- Select the import file or enter the name of the import file in the **File name** field.

4 Importing work systems (optional)

- If the import file contains work systems, then these can also be imported if required. To do this, activate the **Import with work system** check box.

5 Confirming and importing the selection

- Click **[Open]** to confirm the selection.

The operating procedure and method are imported into the OMNIS Software.

NOTICE

If the import file contains prediction models and slope/y-intercept corrections, then these will also be imported.

See also

Exporting operating procedure and method (chapter 5.9.1.6, page 272)

Operating procedure – Definition (chapter 5.9.1, page 260)

Method – Definition (chapter 5.9.2, page 281)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Creating and editing a method (chapter 5.9.2.3, page 284)

Importing the templates (chapter 3.2, page 11)

5.9.1.6 Exporting operating procedure and method

1 Selecting an operating procedure or method

- To export operating procedures and associated methods, click in **Processes ▶ Operating procedures** on .
- To export methods, click in **Processes ▶ Methods** on .

The **Export method / operating procedure** window opens.

2 Selecting or entering a target folder

- Select the target folder or enter the absolute path in the address bar to which the file to be exported will be saved.

3 Defining a file name (optional)

- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

4 Exporting work systems (optional)

- If the export file contains work systems, then these can also be exported if required. To do this, activate the **Export with work system** check box.

5 Creating an export file

- Click **[Save]**, to create the export file.

The operating procedures and methods are exported into the desired folder.

NOTICE

If the export file contains prediction models and slope/y-intercept corrections, then these will also be exported.

See also

Importing operating procedure and method (chapter 5.9.1.5, page 271)

Operating procedure – Definition (chapter 5.9.1, page 260)

Method – Definition (chapter 5.9.2, page 281)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.1.7 Restoring operating procedure and associated methods

1 Opening a sample list

- In **Samples ▶ Sample lists**, select the desired sample list and open it with a double-click.

2 Selecting the 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** working area.

NOTICE

If the restored operating procedure contains prediction models and slope/y-intercept corrections, then these will also be restored.

NOTICE

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

Operating procedure – Definition (chapter 5.9.1, page 260)

Method – Definition (chapter 5.9.2, page 281)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Creating and editing a method (chapter 5.9.2.3, page 284)

Sample list – Tab (chapter 5.2.3, page 100)

Importing operating procedure and method (chapter 5.9.1.5, page 271)

5.9.1.8 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

Editing subsample data (chapter 5.9.1.8.1, page 275)

Importing subsample data (chapter 5.8.5.6, page 197)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

5.9.1.8.1 Editing subsample data

Prerequisite:

- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Opening an operating procedure

- Click in **Processes ▶ Operating procedures** to open 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 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**.

NOTICE

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.

NOTICE

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 desired type (**Text**, **Number**, **Date** or **Selection list**) for the information in the **Type of input field** field.
- Select the desired 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**)

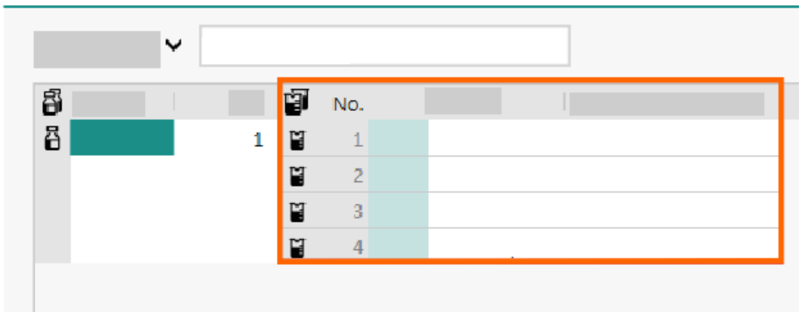
- Depending on the type and use of the input field, additional fields are displayed in the **Properties input field** section that can be filled out as required:
  - For fields of the **Text** type: **Default value**
  - For fields of the **Number** type: **Default value**, **Minimum value**, **Maximum value**, **Unit**
  - For fields of the **Date** type: **Default value**
  - For fields of the **Selection list** type: **List elements**, **Default value**
- Deactivate the **Editable field** check box if the user should be able to edit the input field for the subsample in the sample list.

NOTICE

The option of marking a field as editable or the entire **Properties input field** section is not available in the following cases:

- If **Text** or **Number** was selected in **Type of input field** or 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**.
- If **Selection list** was selected in **Type of input field**.

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 desired 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 5.9.1.3, page 265)

Creating and editing a sample profile (chapter 5.8.4.1, page 176)

Creating samples (chapter 5.8.3.1, page 171)

Carrying over weighing data to subsamples (chapter 5.8.5.3, page 186)

5.9.1.9 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

Run in case of a limit value violation – Definition (chapter 5.9.3.3, page 293)

NOTIFY – Parameters (chapter 5.9.4.16.7, page 599)

Recording the result monitoring (chapter 5.9.1.9.1, page 278)

5.9.1.9.1 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 (x) 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.

NOTICE

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.

NOTICE

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.

NOTICE

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.

NOTICE

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.

NOTICE

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 5.9.1.3, page 265)

NOTIFY – Parameters (chapter 5.9.4.16.7, page 599)

Filtering Search queries (chapter 5.8.2.3, page 167)

Monitoring – Definition (chapter 5.8.22, page 251)

5.9.2 Method – Definition

A **method** is understood to be a combination of commands that can be aligned sequentially and in parallel. Before a method can be used for the analysis of subsamples, it must fulfill the following conditions:

- The method must be assigned a **work system**.
- 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 amount of times saved methods can be used in various operating procedures at the same time.

See also

Operating procedure – Definition (chapter 5.9.1, page 260)

Commands – Definition (chapter 5.9.4, page 293)

Creating and editing a method (chapter 5.9.2.3, page 284)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

5.9.2.1 Methods – Subsection

The following functions are available in **Processes ▶ Method**:

- Use **Create method** to create a new method in which commands can be inserted and edited.
- Use **Import methods** to import one or multiple methods. If the import files contain OMNIS methods and work systems, then these can also be imported.
- Use **Export methods** to export the method as a file. The work systems used in the method can be added to the export file.
- Use **Create parameter report** to create a parameter report for the selected method.
- Use **Duplicate method** to duplicate the method under the same name. The new method contains the same commands, parameters and optional runs as the original method.
- The properties of the selected element are displayed in the **Properties** window.
- Use **Delete method** to delete the method. If the method is used in an operating procedure, the reference to the deleted method will be displayed crossed out in red. The reference will have to be deleted from the operating procedure in order for it to be executed.

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.
Saved	Time at which the method was last saved.
Version	Version number of the object. A new version is created automatically each time the object is saved.
Tags	Existing tags assigned to this method.

See also

Exporting operating procedure and method (chapter 5.9.1.6, page 272)

Filtering operating procedures and methods (chapter 5.9.1.4, page 270)

Importing operating procedure and method (chapter 5.9.1.5, page 271)

Operating procedure and method – Tab (chapter 5.2.6, page 108)

Method – Definition (chapter 5.9.2, page 281)

Method – Properties (chapter 5.9.2.2, page 283)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.2.2 Method – Properties

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**:

NOTICE

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.

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: *Creating a method variable (see chapter 5.9.2.4, page 290)*

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: *Assigning functional units to a command (see chapter 5.10.2.3, page 706)*

Signatures

NOTICE

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.

Further information on signatures:

- *Creating a signature (see chapter 5.6.1, page 132)*
- *Deleting a signature (see chapter 5.6.3, page 135)*
- *Displaying a signature (see chapter 5.6.2, page 134)*

See also

Creating and editing a method (chapter 5.9.2.3, page 284)

Variables – Directory (chapter 5.9.5.3, page 640)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

Assigning functional units to a command (chapter 5.10.2.3, page 706)

5.9.2.3 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**.

NOTICE

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 **Properties ▶ General** in the **Name** field.

NOTICE

The following characters are not allowed: **.|'"{}**

3 Assigning work systems

- Activate the check box for the method to assign the desired work systems in **Properties ▶ Execute with**.

NOTICE

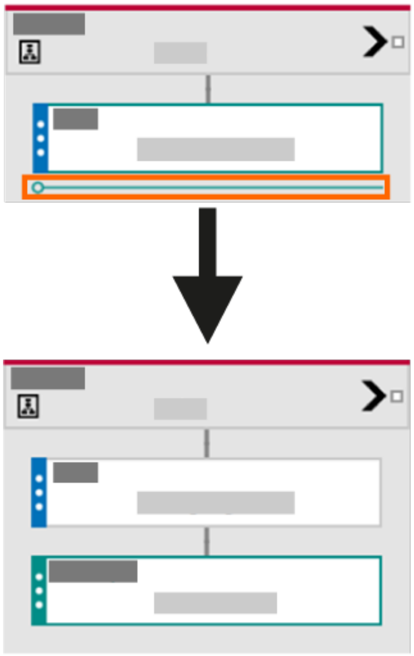
You should select only work systems which can be used to execute the method. This step can also be executed after inserting the commands.

4 Inserting commands

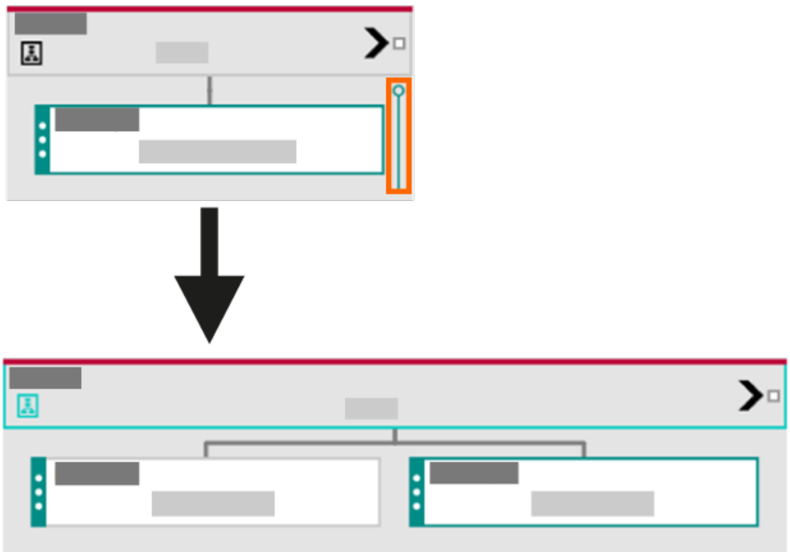
- Click on to open the **Library** window.
- Use drag and drop to insert the desired commands into the method in **Library ▶ Commands**.

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.



NOTICE

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 removed 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.

5 Naming or renaming a command

- Select the desired command.
- Click on to open the **Properties** window.
- Enter the desired name in **Properties** ▶ **General** in the **Name** field.

6 Editing command parameters

- Select the desired command.
- Click on to open the **Properties** window.
- Change the desired command parameter in **Properties** ▶ **Parameters**.

7 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.

NOTICE

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.

8 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.

NOTICE

An optional run can be inserted only parallel to the standard run. Further information on the optional runs:

Run in case of a stop – Definition (see chapter 5.9.3.2, page 292)

Run in case of an error – Definition (see chapter 5.9.3.1, page 291)

9 Validating a method (optional)

- Click on to start the method validation.

NOTICE

We recommend always validating the method before saving it so that any potential problems are immediately identified. 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.

10 Saving a method

- Save the method by clicking on 💾. The method is automatically validated during saving.

NOTICE

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). Then 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 saving the method.

The method is saved. The version and change date of the method are updated automatically in **Properties ▶ General**.

See also

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Creating a work system (chapter 5.10.3.2, page 785)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

Assigning functional units to a command (chapter 5.10.2.3, page 706)

5.9.2.4 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***Creating and editing a method (see chapter 5.9.2.3, page 284)*.

  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.

NOTICE

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

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Creating a work system (chapter 5.10.3.2, page 785)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

Assigning functional units to a command (chapter 5.10.2.3, page 706)

5.9.3 Optional runs

5.9.3.1 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.

NOTICE

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 5.9.2, page 281)

Run in case of a stop – Definition (chapter 5.9.3.2, page 292)

Operating procedure – Definition (chapter 5.9.1, page 260)

5.9.3.2 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.

NOTICE

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 5.9.2, page 281)

Run in case of an error – Definition (chapter 5.9.3.1, page 291)

Operating procedure – Definition (chapter 5.9.1, page 260)

5.9.3.3 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 is violated during a determination with result monitoring, 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.

NOTICE

All optional **Execute on limit** runs defined in the operating procedure are listed in the **Action** selection list in **Result monitoring**.

See also

Operating procedure – Definition (chapter 5.9.1, page 260)

Result monitoring – Definition (chapter 5.9.1.9, page 278)

Recording the result monitoring (chapter 5.9.1.9.1, page 278)

NOTIFY – Parameters (chapter 5.9.4.16.7, page 599)

5.9.4 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 abbreviated designation is in English for all languages) and cannot be changed.
- **Command name**
  Each command has a freely selectable command name.

NOTICE

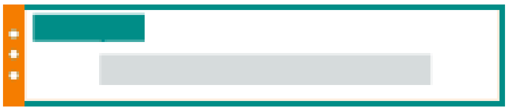
If a command is renamed afterwards, the cross-references to this command (e.g. command variables) are adjusted automatically within the operating procedure and methods.

Representation

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 method run (e.g. branches and loops)
- 

  Dosing commands, automation commands and other commands

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.

NOTICE

All the commands that have more than 1 variable are featured in a separate topic that contains information on their variables.

See also

Operating procedure – Definition (chapter 5.9.1, page 260)

Method – Definition (chapter 5.9.2, page 281)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.1 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 name of the command (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.
Object ID	Display the identification number of the command.

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.

NOTICE

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.

NOTICE

Further information on assigning functional units: *Assigning functional units to a command (see chapter 5.10.2.3, page 706)*

See also

Creating and editing a method (chapter 5.9.2.3, page 284)

Variables – Directory (chapter 5.9.5.3, page 640)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

Assigning functional units to a command (chapter 5.10.2.3, page 706)

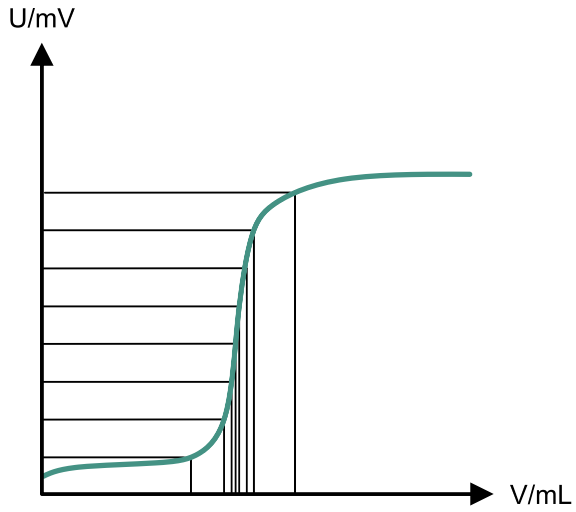
5.9.4.2 Titration commands

5.9.4.2.1 DET – Dynamic equivalence point titration

5.9.4.2.1.1 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.

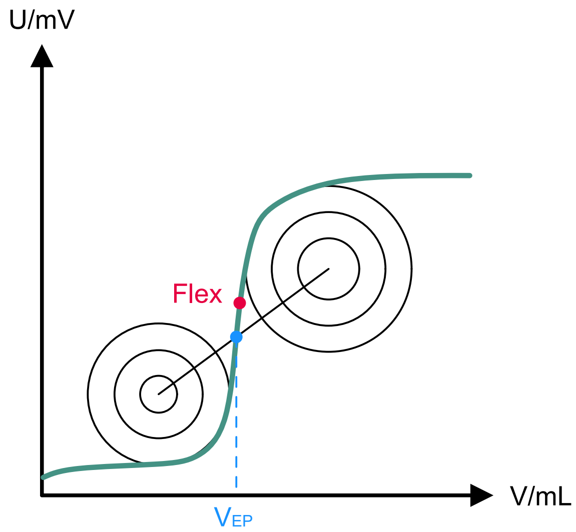


NOTICE

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

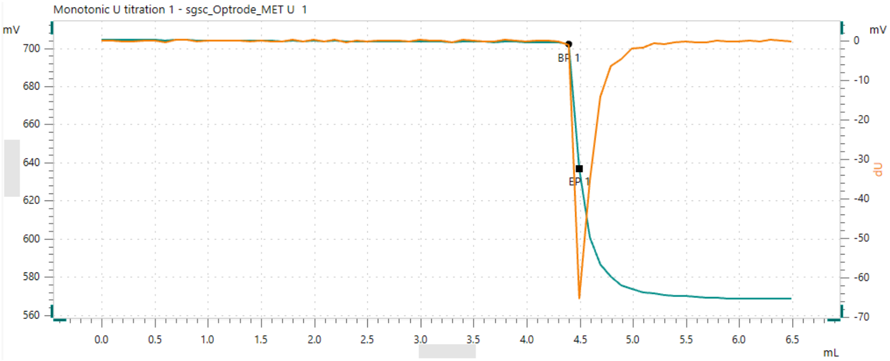
Equivalence points **EP** are evaluated automatically and are determined in a manner similar to that of the Tubbs method. With asymmetric titration curves, the volume value of the equivalence point $\mathbf{V_{EP}}$ is corrected by the inflection point **Flex** in the direction of the smaller circle 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.

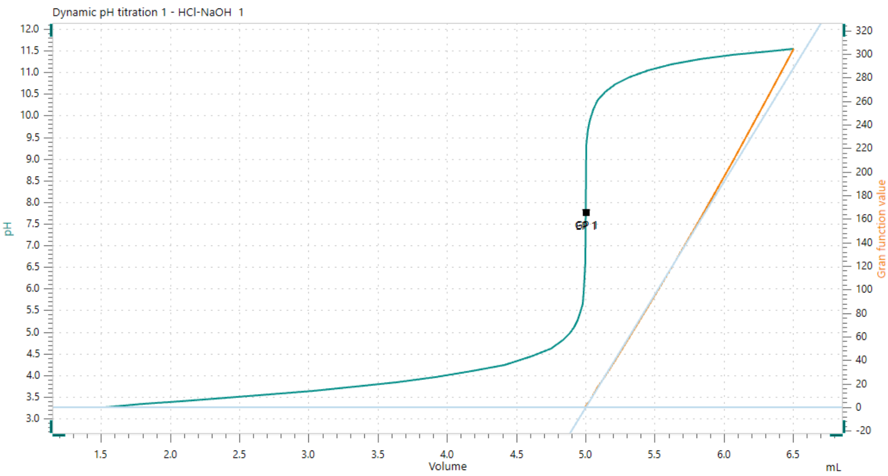
Break point evaluation

A break point evaluation is used to determine sharp changes of direction in the titration curve. This evaluation is suitable for photometric titrations.



Gran evaluation

The equivalence point is determined by the linearization of the titration curve at the time of the Gran evaluation. 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. It is not mandatory to titrate via the equivalence point for an evaluation.



NOTICE

Additional information regarding the Gran evaluation: *Curves – Gran evaluation (see chapter 5.8.15, page 235)*

See also

DET – Properties (chapter 5.9.4.2.1.2, page 299)

DET – Command variables (chapter 5.9.4.2.1.4, page 318)

5.9.4.2.1.2 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 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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 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**.

Start conditions	
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 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	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** deactivates 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 canceled without this start condition having been fulfilled.

Start conditions	
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** deactivates this start condition.
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 with 3 pre-defined 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 pre-defined 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** deactivates 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.
Minimum waiting time	If drift control is activated, 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 activated:** 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 deactivated:** The measured value is adopted after the maximum waiting time has expired.

Titration parameters	
Measuring point distance	The smaller the selected interval between measuring points, 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 interval between measuring points is particularly recommended for steep potential jumps (e.g. for strong acids or bases). The greater the selected interval between measuring points, the larger the volume increments and the faster the titration. A greater interval between measuring points 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.
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.

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.
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.
I(pol) DC (only 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, we recommend 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 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 that 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 dosing 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** deactivates 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 deactivated). **Off** deactivates this stop condition.
Stop EP	The titration is canceled as soon as the specified number of equivalence points (EP) has been evaluated according to the **EP criterion** parameter. **Off** deactivates this stop condition.
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** deactivates 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: *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*.

Potentiometric evaluation	
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. *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*

Fixed point evaluation	
Define fixed points	The window for defining the fixed points is opened. *Curves – Fixed point evaluation (see chapter 5.8.13, page 233)*

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 **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: *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*.
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. *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*

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: *Curves – Gran evaluation (see chapter 5.8.15, page 235)*

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: – **Display regression line** Only valid for **DET U**: ▪ **Potential** Valid for all commands: ▪ **Volume** (default value) ▪ **ERC** ▪ **Time** ▪ **Temperature**
Display regression line	Display of the regression line that runs through the values of the selected quantity. The regression line is activated via the check box. The regression line is displayed only if the quantity **Gran function value** is selected for the y-axis and the quantity **Volume** is selected for the x-axis. The display of the regression line is deactivated by default.

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: – **Display regression line** Only valid for **DET U**: ▪ **Potential** (default value) Valid for all commands: ▪ **Volume** ▪ **ERC** ▪ **Time** ▪ **Temperature**
Display regression line	Display of the regression line that runs through the values of the selected quantity. The regression line is activated via the check box. The regression line is displayed only if the quantity **Gran function value** is selected for the y-axis and the quantity **Volume** is selected for the x-axis. The display of the regression line is deactivated by default.

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: – **Display regression line** Only valid for **DET U**: ▪ **Potential** Valid for all commands: ▪ **Volume** ▪ **ERC** (default value) ▪ **Time** ▪ **Temperature**
Display regression line	Display of the regression line that runs through the values of the selected quantity. The regression line is activated via the check box. The regression line is displayed only if the quantity **Gran function value** is selected for the y-axis and the quantity **Volume** is selected for the x-axis. The display of the regression line is deactivated by default.

Curve simulation	
Curve selection	Simulated curves can be used for 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 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).

NOTICE

The curve simulation cannot be used for instruments of the **Titrando** and **855 Robotic Titrosampler** type.

NOTICE

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 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 **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 5.9.4, page 293)

DET – Run (chapter 5.9.4.2.1.3, page 317)

DET – Command variables (chapter 5.9.4.2.1.4, page 318)

DET – Principle (chapter 5.9.4.2.1.1, page 296)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

Curves – Window-based evaluation (chapter 5.8.12, page 230)

Curves – Fixed point evaluation (chapter 5.8.13, page 233)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

Creating and editing a method (chapter 5.9.2.3, page 284)

Sensor – Definition (chapter 5.10.5, page 794)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

5.9.4.2.1.3 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.

NOTICE

A running titration can be canceled in case of an error, by a manual cancellation or with the emergency stop.

See also

DET – Principle (chapter 5.9.4.2.1.1, page 296)

DET – Properties (chapter 5.9.4.2.1.2, page 299)

DET – Command variables (chapter 5.9.4.2.1.4, page 318)

5.9.4.2.1.4 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.

Command variables
'**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
'**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.
'**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.
'**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

Command variables
'**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.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 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

NOTICE

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.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*' Unit of the concentration of the solution that is dosed with the dosing unit (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 Liquid Adapter and that is dosed with the dosing unit.

Equipment variables
'**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 – Run (chapter 5.9.4.2.1.3, page 317)

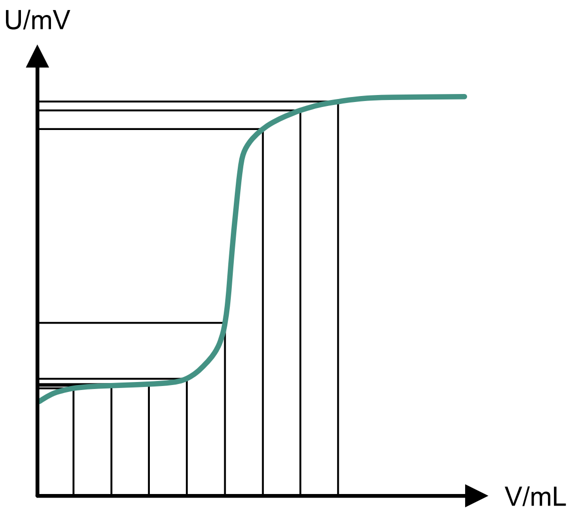
DET – Properties (chapter 5.9.4.2.1.2, page 299)

5.9.4.2.2 MET – Monotonic equivalence point titration

5.9.4.2.2.1 MET – Principle

Measuring principle

Titrations with constant reagent addition are carried out with the **MET** command. The measured values are applied either drift-controlled (equilibrium titration) or after a defined waiting time.



NOTICE

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

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

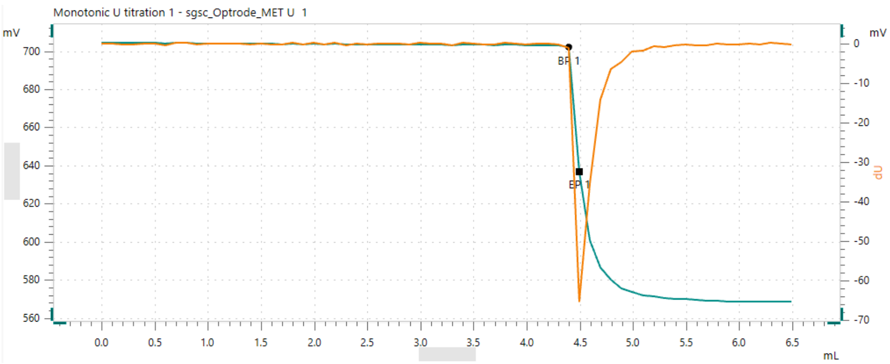
The set EP criterion is compared to the found **ERC** (**E**quivalence point **R**ecognition **C**riterion) for the recognition of the EPs that are found. The ERC is the sum of the measured value changes before and after the jump:

$$|\Delta_{n-2}|+|\Delta_{n-1}|+|\Delta_n|+|\Delta_{n+1}|+|\Delta_{n+2}|$$

In certain cases only three or only one summand is taken into account. EPs with an ERC smaller than the set EP criterion will not be recognized.

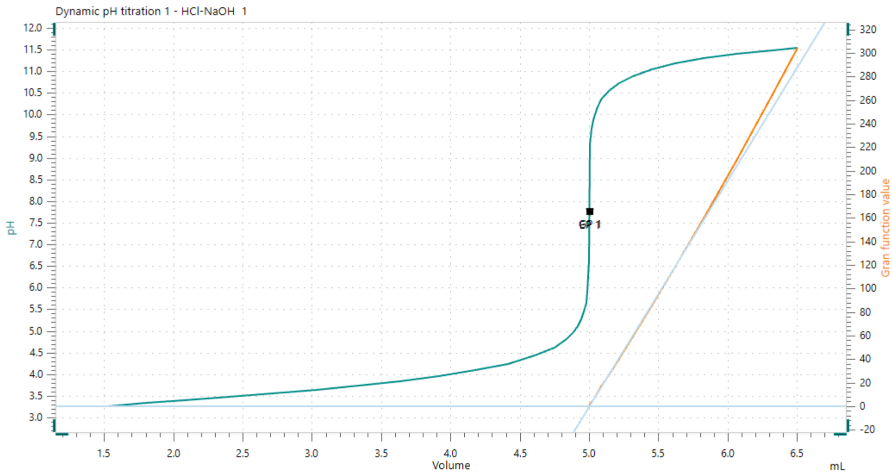
Break point evaluation

A break point evaluation is used to determine sharp changes of direction in the titration curve. This evaluation is suitable for photometric titrations.



Gran evaluation

The equivalence point is determined by the linearization of the titration curve at the time of the Gran evaluation. 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. It is not mandatory to titrate via the equivalence point for an evaluation.



NOTICE

Additional information regarding the Gran evaluation: *Curves – Gran evaluation (see chapter 5.8.15, page 235)*

See also

MET – Properties (chapter 5.9.4.2.2.2, page 324)

MET – Command variables (chapter 5.9.4.2.2.4, page 342)

5.9.4.2.2.2 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 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.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the commands **MET Ipol**, **MET pH** and **MET 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 and the initial measured value is adopted after the maximum waiting time.
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 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** deactivates 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 canceled 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 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	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** deactivates 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 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 with 3 pre-defined 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 pre-defined 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** deactivates 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.

Titration parameters	
Minimum waiting time	If drift control is activated, 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 activated:** 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 deactivated:** The measured value is adopted after the maximum waiting time has expired.
Volume increment	Volume dosed at each dosing step. High accuracy requires using the correct volume increment. A good guideline 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.
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 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, we recommend 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 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 that 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 dosing 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** deactivates 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 deactivated). **Off** deactivates this stop condition.

Stop conditions	
Stop EP	The titration is canceled as soon as the specified number of equivalence points (EP) has been evaluated according to the **EP criterion** parameter. **Off** deactivates this stop condition.
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** deactivates 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 *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*.
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.

Potentiometric evaluation	
[Edit evaluation windows]	The subsection for defining the evaluation windows is opened. *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*

Fixed point evaluation	
Define fixed points	The subsection for defining the fixed points is opened. *Curves – Fixed point evaluation (see chapter 5.8.13, page 233)*
Specified quantity	Selection of the specified quantity for the evaluation of the fixed point from the measuring point list: 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: *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*.
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 subsection for defining the evaluation windows is opened. *Curves – Window-based evaluation (see chapter 5.8.12, page 230)*

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: *Curves – Gran evaluation (see chapter 5.8.15, page 235)*

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 **MET Ipol**: ▪ **Potential** ▪ **dU** Only valid for **MET pH**: ▪ **pH** ▪ **dpH** ▪ **Gran function value** If **Gran function value** is selected, the following specific parameter appears: – **Display regression line** Only valid for **MET U**: ▪ **Potential** ▪ **dU** Valid for all commands: ▪ **Volume** (default value) ▪ **Time** ▪ **Temperature**
Display regression line	Display of the regression line that runs through the values of the selected quantity. The regression line is activated via the check box. The regression line is displayed only if the quantity **Gran function value** is selected for the y-axis and the quantity **Volume** is selected for the x-axis. The display of the regression line is deactivated by default.

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: 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: – **Display regression line** Only valid for **MET U**: ▪ **Potential** (default value) ▪ **dU** Valid for all commands: ▪ **Volume** ▪ **Time** ▪ Temperature
Display regression line	Display of the regression line that runs through the values of the selected quantity. The regression line is activated via the check box. The regression line is displayed only if the quantity **Gran function value** is selected for the y-axis and the quantity **Volume** is selected for the x-axis. The display of the regression line is deactivated by default.

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 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: – **Display regression line** Only valid for **MET U**: ▪ **Potential** ▪ **dU** (default value) Valid for all commands: ▪ **Volume** ▪ **Time** ▪ **Temperature**
Display regression line	Display of the regression line that runs through the values of the selected quantity. The regression line is activated via the check box. The regression line is displayed only if the quantity **Gran function value** is selected for the y-axis and the quantity **Volume** is selected for the x-axis. The display of the regression line is deactivated by default.

Curve simulation	
Curve selection	Simulated curves can be used for 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 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).

NOTICE

The curve simulation cannot be used for instruments of the **Titrando** and **855 Robotic Titrosampler** type.

NOTICE

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 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 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 **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 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 **Interface coulometry** (MET 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 5.9.4, page 293)

DET – Properties (chapter 5.9.4.2.1.2, page 299)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

Curves – Window-based evaluation (chapter 5.8.12, page 230)

Curves – Fixed point evaluation (chapter 5.8.13, page 233)

MET – Run (chapter 5.9.4.2.2.3, page 341)

MET – Command variables (chapter 5.9.4.2.2.4, page 342)

MET – Principle (chapter 5.9.4.2.2.1, page 322)

Creating and editing a method (chapter 5.9.2.3, page 284)

Sensor – Definition (chapter 5.10.5, page 794)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

5.9.4.2.2.3 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.

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.

NOTICE

A running titration can be canceled in case of an error, by a manual cancellation or with the emergency stop.

See also

MET – Principle (chapter 5.9.4.2.2.1, page 322)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

MET – Command variables (chapter 5.9.4.2.2.4, page 342)

5.9.4.2.2.4 MET – Command variables

The following variables are generated by the commands **MET pH**, **MET U** and **MET 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.

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.
'**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
'**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)

Command variables
'**Measvalue.GP{x}**.*Command name*' (x = 1–9) Measured value of the Gran point.
'**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.
'**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.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

Command variables
'**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

NOTICE

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.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*' Unit of the concentration of the solution that is dosed with the dosing unit (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 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 – Run (chapter 5.9.4.2.2.3, page 341)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

5.9.4.2.3 SET – Endpoint titration

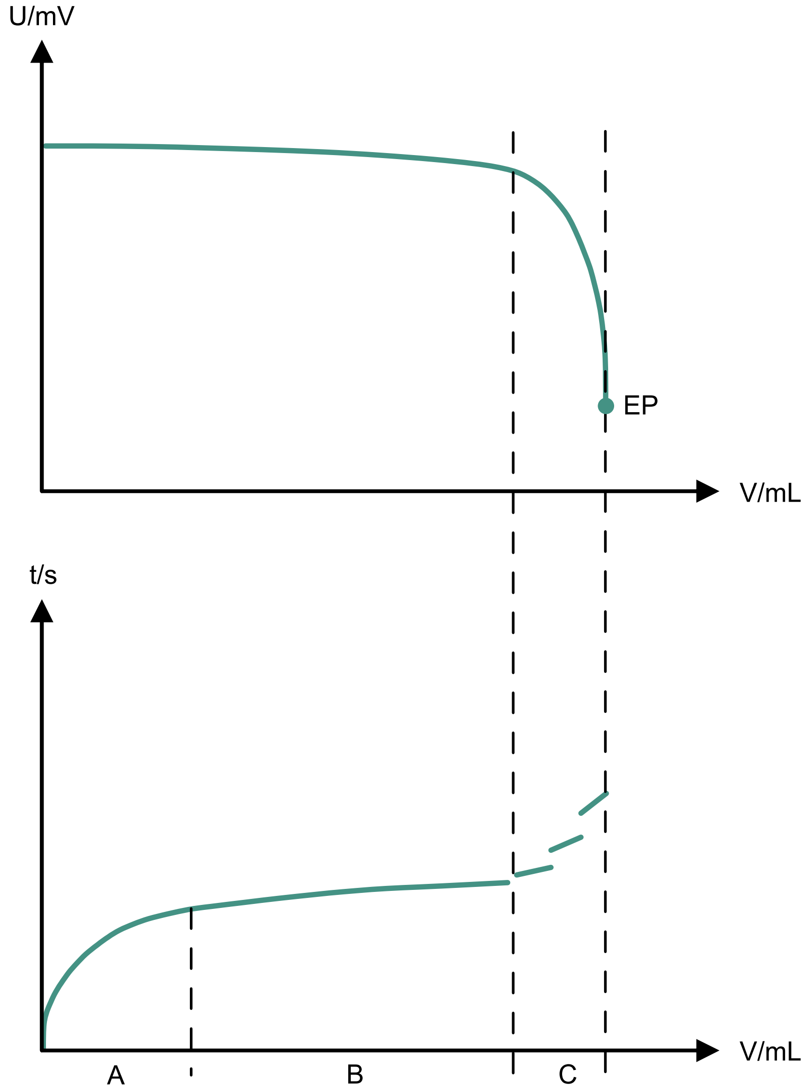
5.9.4.2.3.1 SET – Principle

Principle

The **SET** command is used to carry out titrations to one or two specified endpoints. The titration is canceled at the end point, 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

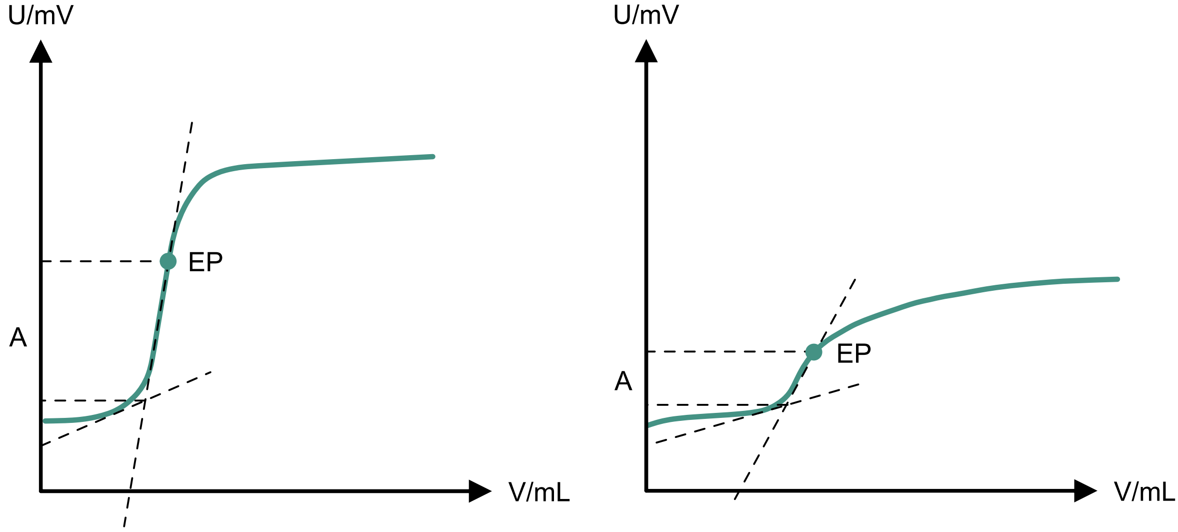
C = Control range

NOTICE

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 – Properties (chapter 5.9.4.2.3.2, page 348)

SET – Command variables (chapter 5.9.4.2.3.4, page 365)

5.9.4.2.3.2 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 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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

NOTICE

The **Parameters for conditioning** are only effective if the endpoint titration is carried out with conditioning. The commands **COND ON** and **COND CHECK** 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 status **Conditioning OK** is reached. The value should be adjusted to the titrant and humidity conditions.

Parameters for conditioning	
Stabilizing time	The **Stabilizing time** starts as soon as the volume drift falls below the **Start drift**. If the volume drift was below the **Start drift** during the entire **Stabilizing time**, the status **Conditioning OK** is reached after the **Stabilizing time** has elapsed. As soon as the volume drift exceeds the **Start drift** during the **Stabilizing time**, the **Stabilizing time** is restarted. If an extraction method with oven is used for the water content determination, Metrohm recommends to increase 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 evaluation 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.
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.

Start conditions	
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, 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 1st endpoint.

Control parameters EP 1	
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. ▪ **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 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 accurate 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.

Control parameters EP 1	
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 1st 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 2nd 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 1st endpoint has been reached and the volume drift falls below the defined **Stop drift**, the endpoint is applied. If a 2nd endpoint has been defined, then the regulated sequence continues to this point, otherwise the titration is ended. ▪ **Delay time**: Once the 1st endpoint has been reached and the selected **Delay time** has passed, the endpoint is applied. If a 2nd 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 2nd endpoint. With **Off**, no titration to the 2nd endpoint will be carried out. ***Note***: If the endpoint titration is carried out with conditioning, the titration to the 2nd endpoint must be deactivated with **Off**.
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. ▪ **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 accurate 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 2nd 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 2nd endpoint has been reached and the volume drift falls below the selected **Stop drift**, the endpoint is applied and the titration is ended.

Control parameters EP 2	
Delay time	Once the 2nd 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 end point 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. When adjusting the polarization current, if necessary, the **Endpoint at** and the **Control range** may have to be adjusted, too.
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 conditioning or titration. It checks within a few seconds whether an electrode is connected and that no short circuit is present. If the titration is carried out with conditioning, then the check is only carried out at the start of 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** deactivates 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** deactivates this stop condition.

Fixed point evaluation	
Define fixed points	The subsection for defining the fixed points is opened. *Curves – Fixed point evaluation (see chapter 5.8.13, page 233)*

Fixed point evaluation	
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 for 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).

NOTICE

The curve simulation cannot be used for instruments of the **Titrando** and **855 Robotic Titrosampler** type.

NOTICE

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 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 **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 5.9.4, page 293)

DET – Properties (chapter 5.9.4.2.1.2, page 299)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

Creating and editing a method (chapter 5.9.2.3, page 284)

Sensor – Definition (chapter 5.10.5, page 794)

SET – Run (chapter 5.9.4.2.3.3, page 363)

SET – Command variables (chapter 5.9.4.2.3.4, page 365)

SET – Principle (chapter 5.9.4.2.3.1, page 346)

5.9.4.2.3.3 SET – Run

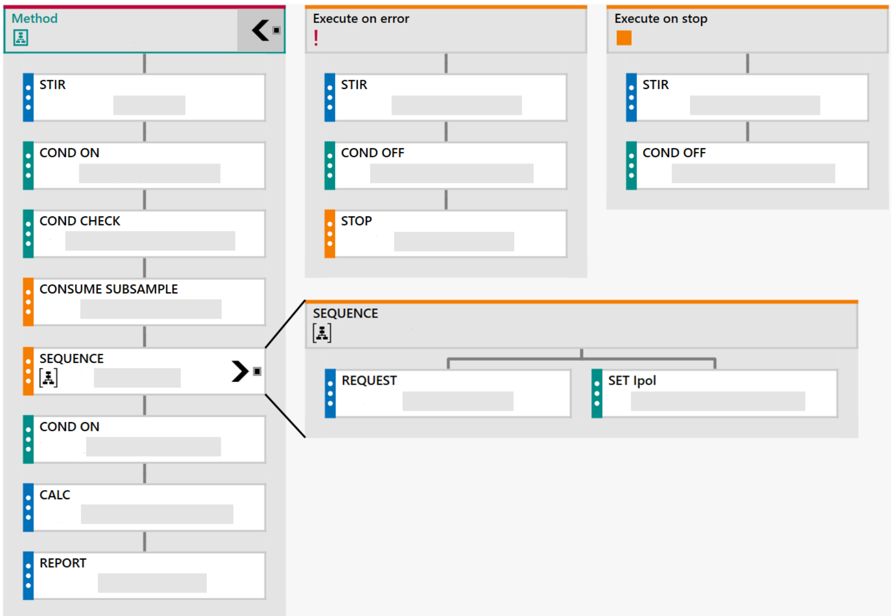
NOTICE

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.

NOTICE

A running titration can be canceled in case of an error, by a manual cancellation or with the emergency stop.

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 subsample. Conditioning can be stopped manually in the window of the respective work system.

See also

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

SET – Command variables (chapter 5.9.4.2.3.4, page 365)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

SET – Principle (chapter 5.9.4.2.3.1, page 346)

5.9.4.2.3.4 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
'**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.
'**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

Command variables
'**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.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.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 correction of the EP volume 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

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

NOTICE

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
'**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 ISE 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

Equipment variables
'**Unit.Concentration.CurrentSolution**.*Command name*' Unit of the concentration of the solution that is dosed with the dosing unit (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 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 ISE electrodes. Unit: Determined by the sensor used.

See also

SET – Run (chapter 5.9.4.2.3.3, page 363)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

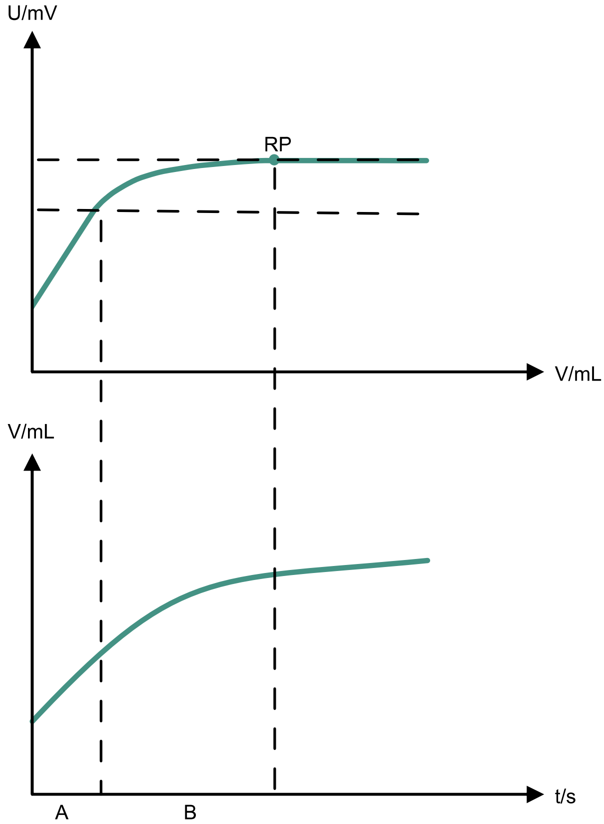
5.9.4.2.4 STAT – Principle

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 immediately titrated off with the titrant, the controller has to 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.



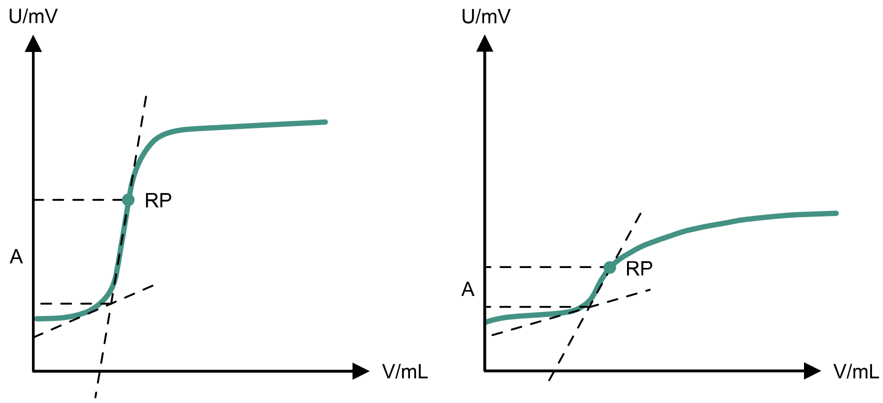
RP = Control point

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

See also

STAT – Run (chapter 5.9.4.2.6, page 379)

STAT – Properties (chapter 5.9.4.2.5, page 371)

STAT – Command variables (chapter 5.9.4.2.7, page 380)

Executing tandem dosing (chapter 5.10.2.14, page 743)

5.9.4.2.5 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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**.

Start conditions	
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.
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.

Control parameters	
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.
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.

Control parameters	
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.
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.

Titration parameters	
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 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. *Curves – Fixed point evaluation (see chapter 5.8.13, page 233)*

Fixed point evaluation	
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**

NOTICE

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: *Executing tandem dosing (see chapter 5.10.2.14, page 743)*

See also

STAT – Run (chapter 5.9.4.2.6, page 379)

STAT – Principle (chapter 5.9.4.2.4, page 369)

STAT – Command variables (chapter 5.9.4.2.7, page 380)

5.9.4.2.6 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.

NOTICE

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.

NOTICE

A running titration can be canceled by a manual cancellation or with the emergency stop or in case of an error.

See also

STAT – Principle (chapter 5.9.4.2.4, page 369)

STAT – Properties (chapter 5.9.4.2.5, page 371)

STAT – Command variables (chapter 5.9.4.2.7, page 380)

5.9.4.2.7 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.
'**Index.FP{x}**.*Command name*' (x = 1–9) Index of the fixed point. Unit: None

Command variables
'**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. 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

NOTICE

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 3rd fixed point).

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.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 ISE 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*' Unit of the concentration of the solution that is dosed with 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 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 ISE electrodes. Unit: Determined by the sensor used.

See also

STAT – Run (chapter 5.9.4.2.6, page 379)

STAT – Principle (chapter 5.9.4.2.4, page 369)

STAT – Properties (chapter 5.9.4.2.5, page 371)

5.9.4.2.8 STDADD ISE – ISE standard addition

5.9.4.2.8.1 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:

$$c_s = \frac{V_s + V_{Add}}{V_s} c_A$$

NOTICE

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**.

NOTICE

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 sizeV_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

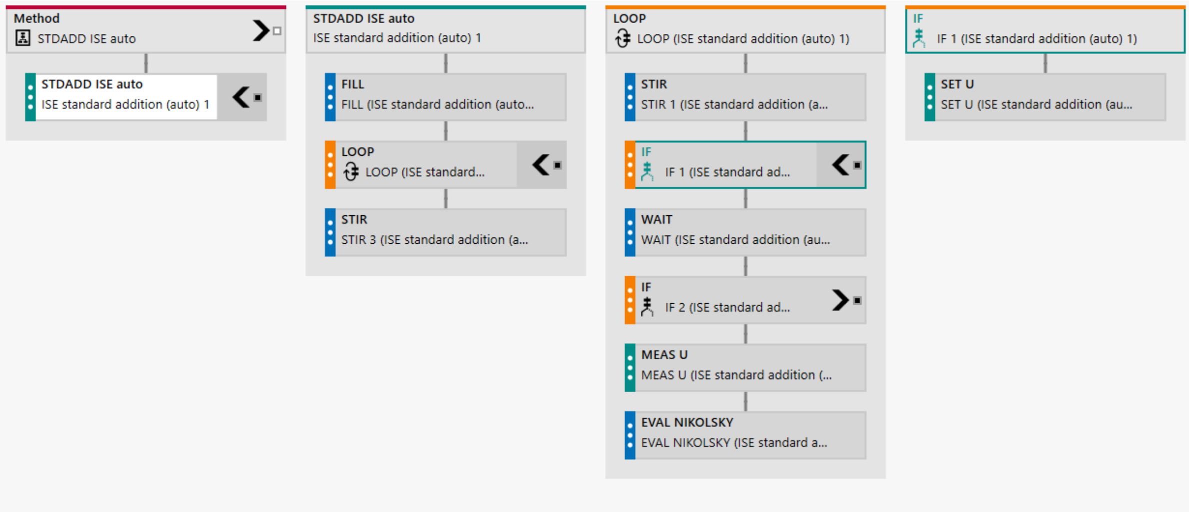
NOTICE

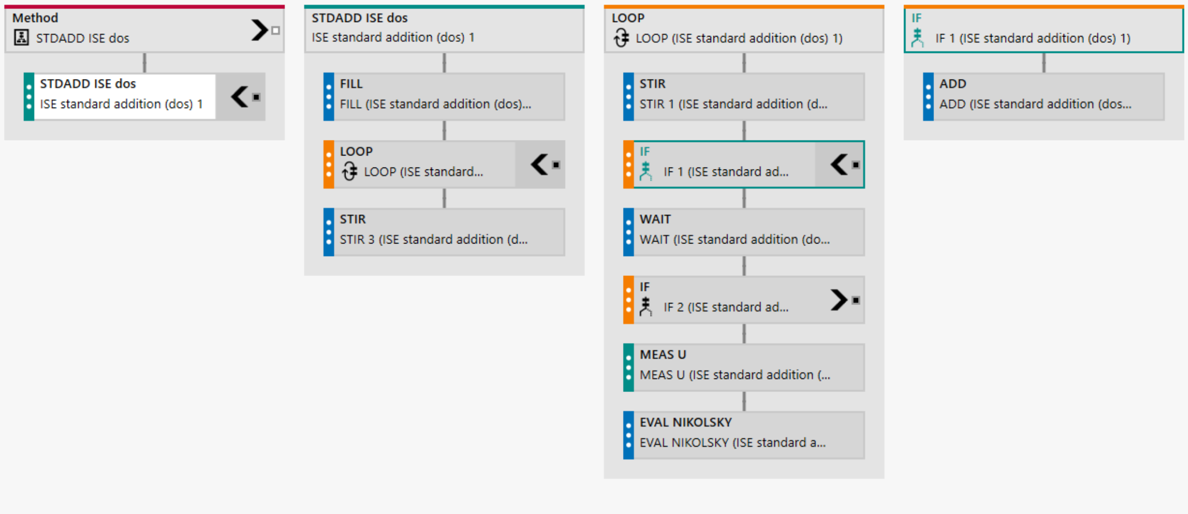
This example is valid for standard additions with any type of ion-selective electrodes.

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.

NOTICE

Further information about the commands contained in **STDADD ISE auto** and **STDADD ISE dos**: *STDADD ISE – Run (see chapter 5.9.4.2.8.3, page 393)*

NOTICE

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 5.9.2.3, page 284)

STDADD ISE – Run (chapter 5.9.4.2.8.3, page 393)

STDADD ISE – Properties (chapter 5.9.4.2.8.2, page 387)

STDADD ISE – Command variables (chapter 5.9.4.2.8.4, page 395)

5.9.4.2.8.2 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 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

Standard addition parameters	
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.
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, we recommend setting the stop volume to the same value as the volume of the buret used.
Stirring time before measurement	Time between the addition of standard solution and the start of the measurement during which stirring takes place, 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 adopted as soon as the signal drift drops below the defined value.

Measuring parameters	
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. ***Note***: This parameter corresponds to the sum of the parameters **Pause before measurement** and **Minimum waiting time** 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 activated, 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.
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 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.

NOTICE

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.

NOTICE

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:

- **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 **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.

NOTICE

Further information on assigning analog sensors: *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)* *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)*

Assigning digital sensors (see chapter 5.10.5.7, page 809)

Assigning analog sensors (see chapter 5.10.5.8, page 811)

See also

STDADD ISE – Principle (chapter 5.9.4.2.8.1, page 383)

STDADD ISE – Run (chapter 5.9.4.2.8.3, page 393)

STDADD ISE – Command variables (chapter 5.9.4.2.8.4, page 395)

5.9.4.2.8.3 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.

NOTICE

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.

NOTICE

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 – Principle (chapter 5.9.4.2.8.1, page 383)

STDADD ISE – Properties (chapter 5.9.4.2.8.2, page 387)

STDADD ISE – Command variables (chapter 5.9.4.2.8.4, page 395)

5.9.4.2.8.4 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** variable category.

NOTICE

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.

'**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

See also

STDADD ISE – Principle (chapter 5.9.4.2.8.1, page 383)

STDADD ISE – Run (chapter 5.9.4.2.8.3, page 393)

STDADD ISE – Properties (chapter 5.9.4.2.8.2, page 387)

5.9.4.2.9 KFT – Volumetric Karl-Fischer titration

5.9.4.2.9.1 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. Depending on the quantity of the water content that needs to be detected, various procedures are used:

- 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 reactants which are 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 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.

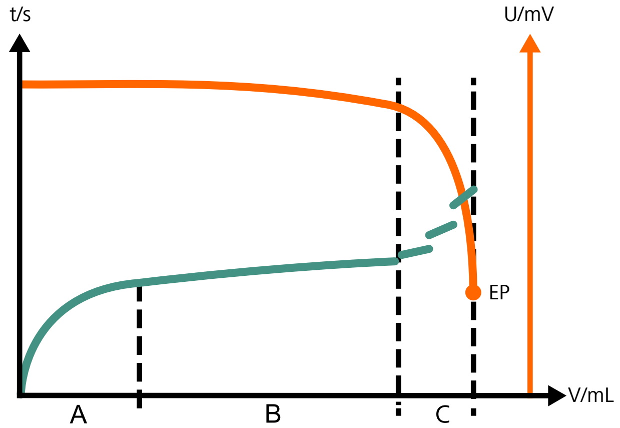


Figure 3 Control curve during a volumetric KF titration

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**.

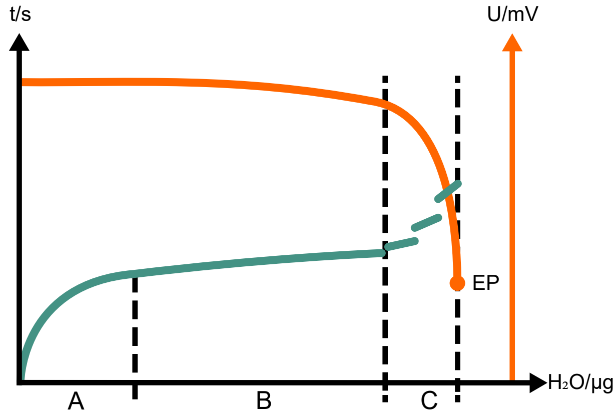


Figure 4 Control curve during a coulometric KF titration

A	**Initial dosing**	**B**	**Continuous dosing**
C	**Control range**	**EP**	**Endpoint**

See also

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

Karl Fischer titration volumetric – Run (chapter 5.9.4.2.9.4, page 415)

KFT – Command variables (chapter 5.9.4.2.9.5, page 418)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Karl Fischer titration coulometric – Run (chapter 5.9.4.2.10.2, page 430)

KFC – Command variable (chapter 5.9.4.2.10.3, page 432)

5.9.4.2.9.2 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***COND ON – Parameters (see chapter 5.9.4.2.12.1, page 440)*: Start conditioning.
- **COND CHECK***COND CHECK – Parameters (see chapter 5.9.4.2.14.1, page 442)*: 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***COND CHECK – Parameters (see chapter 5.9.4.2.14.1, page 442)*. 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.

NOTICE

Further information on the icons that are displayed with the measured values: *Displaying live data and controlling run (see chapter 5.8.9, page 222)*

See also

KFT – Command variables (chapter 5.9.4.2.9.5, page 418)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

SET – Command variables (chapter 5.9.4.2.3.4, page 365)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

5.9.4.2.9.3 Karl Fischer titration volumetric – 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.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **KFT Ipol** command:

Parameters

NOTICE

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 **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 status **Conditioning OK** is reached. The value should be adjusted to the titrant and humidity conditions.

Parameters for conditioning	
Stabilizing time	The **Stabilizing time** starts as soon as the volume drift falls below the **Start drift**. If the volume drift was below the **Start drift** during the entire **Stabilizing time**, the status **Conditioning OK** is reached after the **Stabilizing time** has elapsed. As soon as the volume drift exceeds the **Start drift** during the **Stabilizing time**, the **Stabilizing time** is restarted. Metrohm recommends to set 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 to increase the value to at least 10 s.
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, the titration starts automatically in the **Conditioning OK** status (without waiting for the **Sample addition time** to elapse). In order get 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 *OMNIS Titrator – 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 adapted. ▪ If the **Recognition of sample addition** function is activated, the **Correction with volume drift** must not be set to **Automatic**. ***Note:*** The **Recognition of sample addition** function only exists in OMNIS instruments.
Threshold value	The volume drift must have exceeded the **Threshold value** in a short time in order for the conditioning to stop automatically and for the process sequence to continue from the status **Conditioning OK** 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**, the **Sample addition time** is skipped.

Parameters for conditioning	
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 evaluation 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.
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 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 conditions	
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**
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.

Endpoint control parameters	
Titration rate	The titration rate can either be determined with 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 to use the **Optimal 2-component reagents** rate and enter a value of 20 µA in the **I(pol) DC** parameter.
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 accurate the endpoint is approached. The control range can be reduced if accuracy has a subordinated role and titration should be carried out faster.

Endpoint 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 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.
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 evaluation 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 end point 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 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 devices 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.

Titration parameters	
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 that no short circuit is present. If the titration is carried out with conditioning, then the check is only carried out 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** deactivates 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** deactivates this stop condition.

Fixed point evaluation	
Define fixed points	The subsection for defining the fixed points is opened. *Curves – Fixed point evaluation (see chapter 5.8.13, page 233)*
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 for 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.

NOTICE

Before analyzing real samples, deactivate the curve simulation. No curve simulation is available for instruments of the **Titrando** type.

NOTICE

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** 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 **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

Commands – Definition (chapter 5.9.4, page 293)

COND ON – Parameters (chapter 5.9.4.2.12.1, page 440)

COND CHECK – Parameters (chapter 5.9.4.2.14.1, page 442)

COND OFF – Parameters (chapter 5.9.4.2.13.1, page 441)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

Karl Fischer titration volumetric – Run (chapter 5.9.4.2.9.4, page 415)

KFT – Command variables (chapter 5.9.4.2.9.5, page 418)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.2.9.4 Karl Fischer titration volumetric – Run

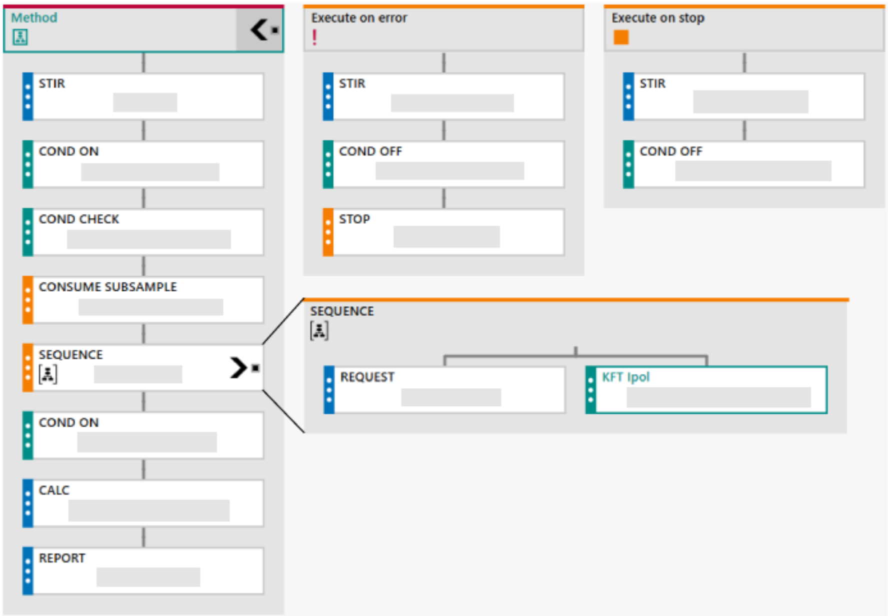
NOTICE

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.

NOTICE

A running titration can be canceled in case of an error, by a manual cancellation or with the emergency stop.

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 5.9.4.2.14.2, page 444)

COND CHECK – Parameters (chapter 5.9.4.2.14.1, page 442)

COND OFF – Parameters (chapter 5.9.4.2.13.1, page 441)

COND ON – Parameters (chapter 5.9.4.2.12.1, page 440)

KFT – Command variables (chapter 5.9.4.2.9.5, page 418)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

5.9.4.2.9.5 KFT – Command variables

The following variables are generated by the **KFT Ipol** command during the process sequence and can be used under the variable category

- **Command variables** or
- **Equipment variables**

as '**Variable name**.*Command name*' in a formula.

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
'**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

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.
'**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
'**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

Command variables
'**Time.EP{1}**.*Command name'* Time stamp associated with the endpoint. 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 correction of the EP volume 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
'**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

NOTICE

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.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
'**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

Karl Fischer titration volumetric – Run (chapter 5.9.4.2.9.4, page 415)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

5.9.4.2.10 KFC – Coulometric Karl Fischer titration

5.9.4.2.10.1 Karl Fischer titration coulometric – Properties

The **KFC** command is a titration command for the **c**oulometric **K**arl **F**ischer titration (KFC). The coulometric water content determination is mainly used to determine small amounts of water.

With **KFC**, the necessary iodine is directly and electrochemically generated in the electrolyte 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.

Clicking on  under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **KFC** command:

Parameters

NOTICE

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 run before the **KFC** command for this purpose.

Parameters for conditioning	
Start drift	The **Start drift** is a threshold value that the amount drift needs to be below during the entire **Stabilizing time** so that the status **Conditioning OK** is reached. The value should be adjusted to the titrant and humidity conditions.

<table>
<tr><th colspan="2">Parameters for conditioning</th></tr>
<tr><td>Stabilizing time</td><td>The Stabilizing time starts as soon as the amount drift falls below the Start drift.

If the amount drift was below the Start drift during the entire Stabilizing time, the status Conditioning OK is reached after the Stabilizing time has elapsed.

As soon as the amount drift exceeds the Start drift during the Stabilizing time, the Stabilizing time is restarted.

Metrohm recommends to set 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 to increase the value to at least 60 s.</td></tr>
<tr><td>Recognition of sample addition</td><td>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, the titration starts automatically in the Conditioning OK status (without waiting for the Sample addition time to elapse).

In order get correct results when working with the Recognition of sample addition, the following preconditions must be met:

▪ The electrodes must be positioned correctly, as described in Mounting the KF titration cell in the product manual of the 851 Titrando (8.851.8004).
▪ The sample in the measuring cell must be well mixed. In order to do so, the stirring rate of the stirrer must be adapted.</td></tr>
<tr><td>Threshold value</td><td>The Potential must have exceeded the Threshold value in a short time in order for the conditioning to stop automatically and for the process sequence to continue from the status Conditioning OK due to the Recognition of sample addition.</td></tr>
<tr><td>Sample addition time</td><td>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 sample into the titration cell.

If the titration was started with Recognition of sample addition, the Sample addition time is skipped.</td></tr>
</table>

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 evaluation 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 leakproof 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 recording of the titration curve is started.

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 with 3 pre-defined 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 pre-defined 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 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 accurate 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 evaluation data.

Titration parameters	
Extraction time	During the **Extraction time**, no end point 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 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) 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	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 that no short circuit is present. If the titration is carried out with conditioning, then the check is only carried out at the start of conditioning.
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** deactivates this stop condition.

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 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** ▪ **Water** ▪ **Potential** ▪ **Drift** (default value) ▪ **Temperature** ▪ **Charge** ▪ **Ugen** ▪ **Igen**

NOTICE

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

Execute with

For a **KFC** command to be executed, the corresponding functional unit and required sensor must be assigned to it.

- Analog measuring input to which the sensor required for the titration is connected:
  Interface coulometry
- Analog sensor:
  Polarizable metal electrode, **pH electrode** or **Temperature sensor**

After a functional unit for the command has been selected, the following additional parameters appear:

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

Commands – Definition (chapter 5.9.4, page 293)

COND CHECK – Parameters (chapter 5.9.4.2.14.1, page 442)

COND CHECK – Command variables (chapter 5.9.4.2.14.2, page 444)

COND OFF – Parameters (chapter 5.9.4.2.13.1, page 441)

COND ON – Parameters (chapter 5.9.4.2.12.1, page 440)

Karl Fischer titration coulometric – Run (chapter 5.9.4.2.10.2, page 430)

KFC – Command variable (chapter 5.9.4.2.10.3, page 432)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.2.10.2 Karl Fischer titration coulometric – Run

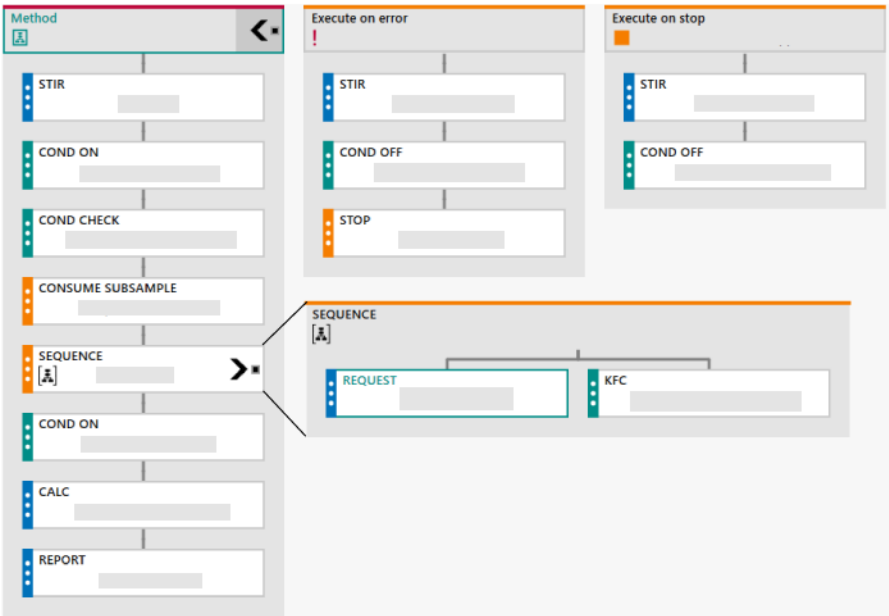
NOTICE

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**.

During the titration:

- **Graph – … 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.

NOTICE

A running titration can be canceled in case of an error or with a manual input.

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 subsample. Conditioning can be stopped manually in the window of the respective work system.

See also

COND CHECK – Command variables (chapter 5.9.4.2.14.2, page 444)

COND CHECK – Parameters (chapter 5.9.4.2.14.1, page 442)

COND OFF – Parameters (chapter 5.9.4.2.13.1, page 441)

COND ON – Parameters (chapter 5.9.4.2.12.1, page 440)

KFC – Command variable (chapter 5.9.4.2.10.3, page 432)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

5.9.4.2.10.3 KFC – Command variable

The following variables are generated by the **KFC** command during the process sequence and can be used as '**Variable name**.*Command name*' under the **Command variables** variable category in a formula.

'**Amount.DriftCorrection**.*Command name*'

Water content that was calculated for the drift-based correction of the EP water content.

The correction water volume is calculated by multiplying the amount drift with the period from the end of conditioning until the end of the titration.

When working with conditioning, this water content 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

'**Amount.EP{1}**.*Command name*'

Water content of the subsample at the endpoint.

Unit: µg

'**Amount.Final**.*Command name*'

Final water content of the subsample after processing the command.

Unit: µg

'**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

'**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 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

'**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

'**Temperature.EP{1}**.*Command name*'

Temperature associated with the endpoint.

Unit: °C

'**Temperature.Final**.*Command name*'

End temperature after processing the command.

Unit: °C

'**Time.EP{1}**.*Command name*'

Time stamp associated with the endpoint.

Unit: s

'**Unit.Measvalue**.*Command name*'

Unit of the measured value.

Unit: mV

See also

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Karl Fischer titration coulometric – Run (chapter 5.9.4.2.10.2, page 430)

5.9.4.2.11 COLLECT – Combining measured values

5.9.4.2.11.1 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.

NOTICE

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: *COLLECT – Concept (see chapter 5.9.4.2.11.2, page 436)*

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.

NOTICE

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.

NOTICE

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

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Commands – Definition (chapter 5.9.4, page 293)

COLLECT – Concept (chapter 5.9.4.2.11.2, page 436)

5.9.4.2.11.2 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**.

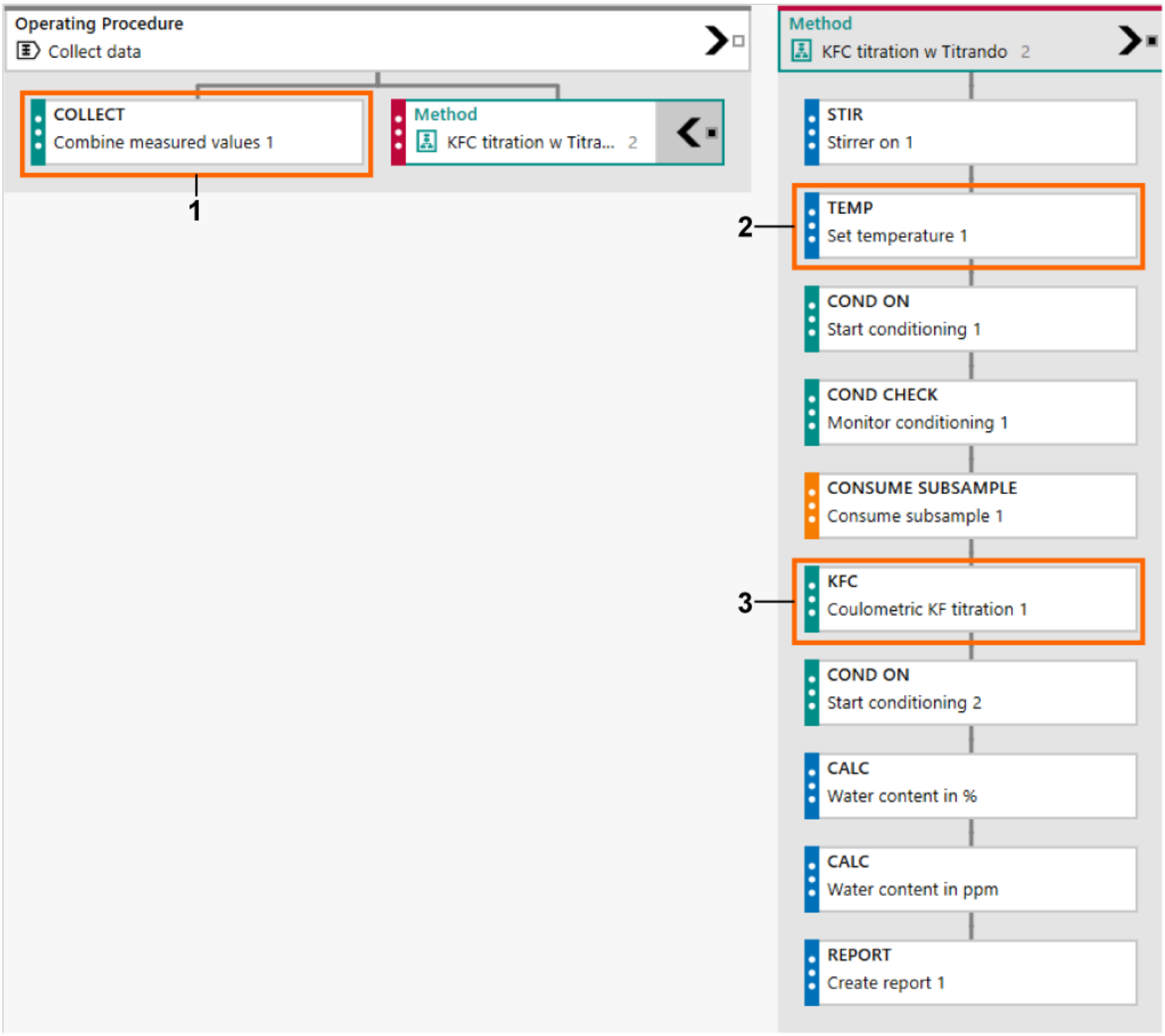
The **COLLECT** command can be inserted anywhere in methods and operating procedures. However, depending on the placement, an incomplete or empty measuring point list may occur.

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 **COLLECT** command must be placed before the primary command.

Example of an operating procedure with COLLECT command

The following example shows a possible arrangement of methods and commands within an operating procedure. Other arrangements and combinations are possible.

This example shows a coulometric Karl Fischer titration with one **KFC** command as primary command and one **TEMP** command as secondary command.



If the **COLLECT** command is inserted in parallel with the method containing the primary command, the following sequence results:

1. The **COLLECT** command **(1)** starts. However, no measuring point list is created yet.
2. The secondary command **(2)** starts. Furthermore, no measuring point list is created.
3. The primary command **(3)** starts. Starting the primary command starts the recording of measuring points from the primary command and measured values from the secondary command.

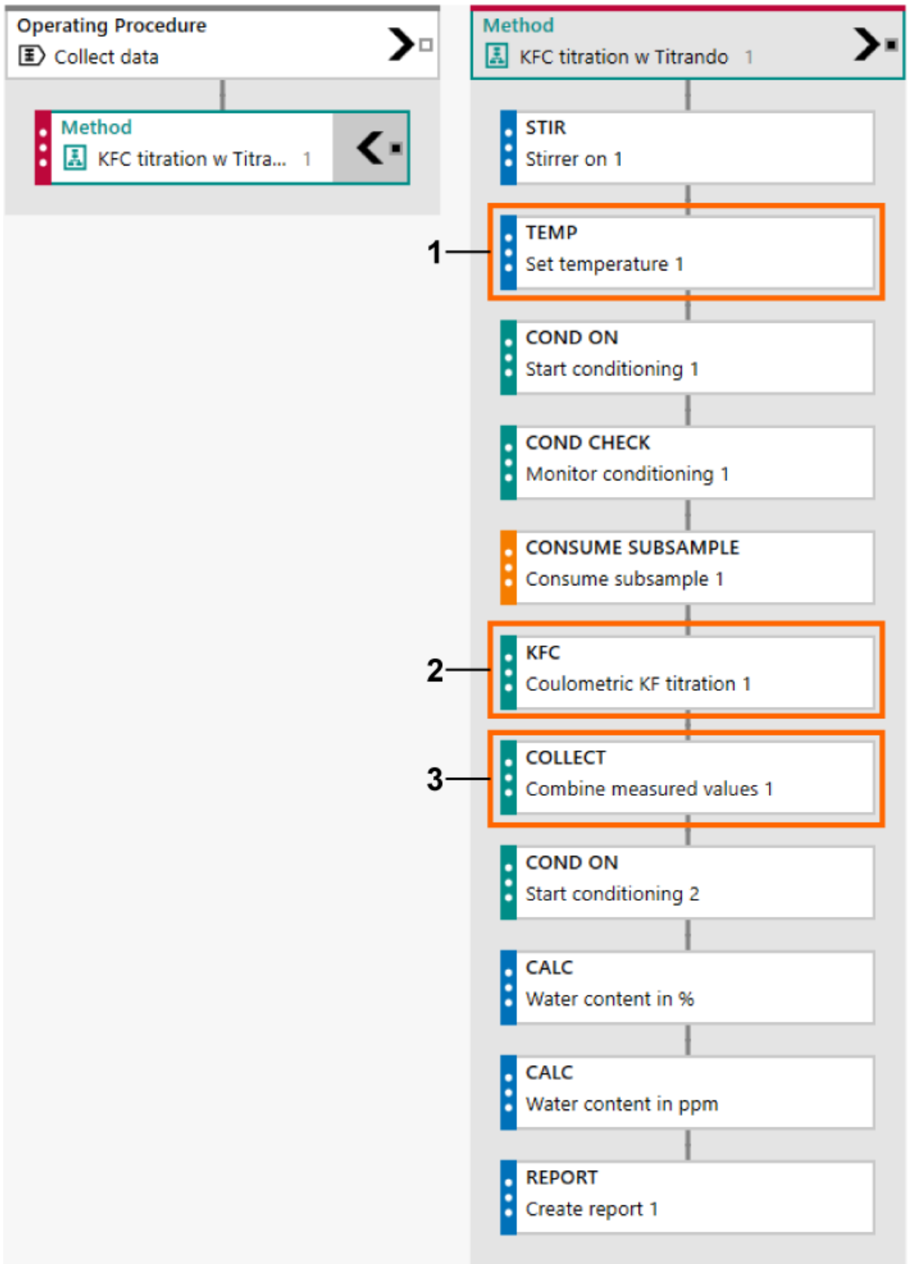
NOTICE

If the **COLLECT** command is placed incorrectly, the command can create no or only an incomplete list of measuring points. The following errors lead to 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.
- A 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**.

Example of an incorrect arrangement

The following example shows a possible arrangement of methods and commands within an operating procedure in which no measuring point list is created by the **COLLECT** command.



1. The secondary command **(1)** starts. No measuring point list is created.
2. The primary command **(2)** starts. No measuring point list with merged measuring points and measured values is created.
3. The primary command is terminated.
4. The **COLLECT** command **(3)** starts. No measuring point list is created as the primary command has already been exited.

See also

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

COLLECT – Parameters (chapter 5.9.4.2.11.1, page 434)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.2.12 COND ON – Starting the conditioning

5.9.4.2.12.1 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 *Karl Fischer titration – Principle (see chapter 5.9.4.2.9.1, page 397)*
Karl Fischer titration – Principle (see chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (see chapter 5.9.4.2.9.2, page 402).

NOTICE

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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

Karl Fischer titration volumetric – Run (chapter 5.9.4.2.9.4, page 415)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

KFT – Command variables (chapter 5.9.4.2.9.5, page 418)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Karl Fischer titration coulometric – Run (chapter 5.9.4.2.10.2, page 430)

COND CHECK – Parameters (chapter 5.9.4.2.14.1, page 442)

COND OFF – Parameters (chapter 5.9.4.2.13.1, page 441)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.2.13 COND OFF – End conditioning

5.9.4.2.13.1 COND OFF – Parameters

The **COND OFF** command stops the conditioning and deactivates the polarization of the electrode (e.g. in case of an error).

NOTICE

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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

Karl Fischer titration volumetric – Run (chapter 5.9.4.2.9.4, page 415)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

KFT – Command variables (chapter 5.9.4.2.9.5, page 418)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

COND ON – Parameters (chapter 5.9.4.2.12.1, page 440)

Karl Fischer titration coulometric – Run (chapter 5.9.4.2.10.2, page 430)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.2.14 CONDCHECK – Monitoring conditioning

5.9.4.2.14.1 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.

NOTICE

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 *Karl Fischer titration volumetric – Properties (see chapter 5.9.4.2.9.3, page 404)*. 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.

NOTICE

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

See also

Commands – Definition (chapter 5.9.4, page 293)

CAL COND – Properties (chapter 5.9.4.13.3, page 521)

Karl Fischer titration coulometric – Run (chapter 5.9.4.2.10.2, page 430)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Karl Fischer titration volumetric – Run (chapter 5.9.4.2.9.4, page 415)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

Creating and editing a method (chapter 5.9.2.3, page 284)

SET – Run (chapter 5.9.4.2.3.3, page 363)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

5.9.4.2.14.2 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 '**Measvalue.Final**.*Command name*'

Variables for the KFC command

Command variables
'**Amount.Conditioning**.*Command name*' Water quantity for the conditioning. 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 subsample addition to subsample 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 5.9.4.2.14.1, page 442)

Karl Fischer titration coulometric – Run (chapter 5.9.4.2.10.2, page 430)

KFC – Command variable (chapter 5.9.4.2.10.3, page 432)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Karl Fischer titration volumetric – Run (chapter 5.9.4.2.9.4, page 415)

KFT – Command variables (chapter 5.9.4.2.9.5, page 418)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)
Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

SET – Run (chapter 5.9.4.2.3.3, page 363)

SET – Command variables (chapter 5.9.4.2.3.4, page 365)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

5.9.4.3 PREDICT – Parameters

The **PREDICT** command is used to evaluate a measured spectrum with a prediction model. A slope/y-intercept correction can be applied afterwards if required.

The **PREDICT** command is executed with the parameters listed in the following:

Name of the measuring command	Selection of the measuring command that is to be referenced with which the spectrum was acquired.
Prediction model	Selection of the prediction model that is to be used for the evaluation of a spectrum. The last published prediction models are displayed in alphabetical order. Additional information on publishing prediction models: *Publishing a prediction model (see chapter 5.11.1.17, page 903)*
Slope/y-intercept correction	**Optional**: Selection of the slope/y-intercept correction that is to be used after the evaluation of a spectrum. The last published slope/y-intercept corrections are displayed in alphabetical order. By default, no slope/y-intercept correction is used. Additional information on slope/y-intercept corrections: *Slope/y-intercept correction – Definition (see chapter 5.11.2.7, page 915)*

NOTICE

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

See also

PREDICT – Command variables (chapter 5.9.4.3.1, page 448)

MEAS SPEC – Properties (chapter 5.9.4.12.7, page 502)

Creating and editing a method (chapter 5.9.2.3, page 284)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

5.9.4.3.1 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.

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.Result**.*Command name*' Assessment of the predicted result as an outlier. ▪ **1**: The result is an outlier. ▪ **2**: The result is **not** an outlier.
'**HotellingsT2.Result**.*Command name*' Calculated result value (Hotelling's T^2). Unit: Defined in the 'Unit.Result' variable
'**QResiduals.Result**.*Command name*' Calculated result value (Q residuals). Unit: Defined in the 'Unit.Result' variable
'**Result**.*Command name*' Predicted final value. If a slope/y-intercept correction is used, the result will be corrected with this. Unit: Defined in the 'Unit.Result' variable
'**Unit.Result**.*Command name*' Unit of the result. It is defined by the user in the properties of the referenced prediction model in **Models ► Prediction models ► Spectra list** in the **Reference parameter/unit** field.
'**Uncorrected.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

See also

PREDICT – Parameters (chapter 5.9.4.3, page 447)

5.9.4.4 VAL WL – Properties

The **VAL WL** command is used to validate a wavelength calibration and bandwidth calibration of a spectrometer carried out with the **CAL WL** command.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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)

Execute with

For a **VAL WL** command to be executed, an instrument of the **2060 the NIR** type must be assigned.

See also

Creating and editing a method (chapter 5.9.2.3, page 284)

VAL WL – Command variables (chapter 5.9.4.4.1, page 450)

CAL WL – Properties (chapter 5.9.4.8, page 459)

CAL WL – Command variables (chapter 5.9.4.8.1, page 460)

5.9.4.4.1 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
'**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

VAL WL – Properties (chapter 5.9.4.4, page 449)

CAL WL – Properties (chapter 5.9.4.8, page 459)

CAL WL – Command variables (chapter 5.9.4.8.1, page 460)

5.9.4.5 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).

Clicking on under **Processes** ► **Method** ► **Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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 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, 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.

Measuring parameters	
Reflection standard	Selection of the external NIR reflection standard that is used for the validation of the reference standardization. Further information on the standards: *Standards – Subsection (see chapter 5.10.10, page 860)*, *Importing standards (see chapter 5.10.10.2, page 862)*

NOTICE

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 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: ▪ **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**

NOTICE

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

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 5.9.2.3, page 284)

VAL REF STD – Command variables (chapter 5.9.4.5.1, page 453)

REF STD – Properties (chapter 5.9.4.6, page 454)

REF STD – Command variables (chapter 5.9.4.6.1, page 457)

Importing standards (chapter 5.10.10.2, page 862)

Standards – Properties / Specific data (chapter 5.10.10.1, page 862)

5.9.4.5.1 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.
'**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
'**OverallStatus.Result**.*Command name*' Overall validation status of the reference standardization. ▪ **1**: The validation was successful. ▪ **2**: The validation failed.

See also

VAL REF STD – Properties (chapter 5.9.4.5, page 451)

REF STD – Properties (chapter 5.9.4.6, page 454)

REF STD – Command variables (chapter 5.9.4.6.1, page 457)

5.9.4.6 REF STD – Properties

The **REF STD** command is used to remove interferences of optical fibers and measuring probes from the absorbance spectrum of the sample. Reference standardization ensures that absorbance values on a certain wavelength range are comparable between different systems.

Clicking on under **Processes ► Method ► Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.
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 parameters	
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. Further information on the standards: *Standards – Subsection (see chapter 5.10.10, page 860)*, *Importing standards (see chapter 5.10.10.2, page 862)*

NOTICE

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 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: ▪ **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**

NOTICE

Further 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 5.9.2.3, page 284)

REF STD – Command variables (chapter 5.9.4.6.1, page 457)

VAL REF STD – Properties (chapter 5.9.4.5, page 451)

VAL REF STD – Command variables (chapter 5.9.4.5.1, page 453)

Importing standards (chapter 5.10.10.2, page 862)

Standards – Properties / Specific data (chapter 5.10.10.1, page 862)

5.9.4.6.1 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 5.9.4.6, page 454)

VAL REF STD – Properties (chapter 5.9.4.5, page 451)

VAL REF STD – Command variables (chapter 5.9.4.5.1, page 453)

5.9.4.7 MEAS REF SPEC – Properties

The **MEAS REF SPEC** command is used to record the reference spectrum for the measurement of samples.

Clicking on under **Processes ► Method ► Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS REF SPEC** command:

Parameters

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.

NOTICE

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

Execute with

For a **MEAS REF SPEC** command to be executed, an instrument of the **2060 the NIR** type must be assigned.

See also

Creating and editing a method (chapter 5.9.2.3, page 284)

MEAS REF SPEC – Command variables (chapter 5.9.4.7.1, page 458)

MEAS SPEC – Properties (chapter 5.9.4.12.7, page 502)

5.9.4.7.1 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**.*Command name*' Time at which the reference spectrum was acquired.

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

MEAS REF SPEC – Properties (chapter 5.9.4.7, page 457)

5.9.4.8 CAL WL – Properties

The **CAL WL** command is used to carry out a wavelength calibration and bandwidth calibration of the spectrometer by assigning the pixels of the spectrometer to a wavelength. The wavelength accuracy of the spectrometer is determined by the difference between the calculated and the actual wavelength position.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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

For a **CAL WL** command to be executed, an instrument of the **2060 the NIR** type must be assigned.

See also

CAL WL – Command variables (chapter 5.9.4.8.1, page 460)

Creating and editing a method (chapter 5.9.2.3, page 284)

VAL WL – Properties (chapter 5.9.4.4, page 449)

VAL WL – Command variables (chapter 5.9.4.4.1, page 450)

5.9.4.8.1 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 5.9.4.8, page 459)

VAL WL – Properties (chapter 5.9.4.4, page 449)

VAL WL – Command variables (chapter 5.9.4.4.1, page 450)

5.9.4.9 TEST NOISE – Properties

The **TEST NOISE** command is used to test the signal noise of the spectrometer. The RMS noise, the peak-to-peak noise and the baseline bias of 10 spectra in different segments are determined and compared to the tolerance value.

Clicking on under **Processes ▶ Method ▶ Library ▶ Commands** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **TEST NOISE** command:

Parameters

Measuring parameters	
Measuring mode	Selection of the measuring mode. ▪ **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 NIR reflection standard that is used for testing of the signal noise. Further information on the standards: *Standards – Subsection (see chapter 5.10.10, page 860)*, *Importing standards (see chapter 5.10.10.2, page 862)*

NOTICE

10 spectra are recorded per **TEST NOISE** command.

Chart – x-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the x-axis: ▪ **Wavelength** ▪ To display absorbance on the x-axis, one of the following 10 options must be selected: – **Spectrum 1–Spectrum 10**

Chart – y-axis	
Quantity	Selection of the specified quantity to be shown in the curve display on the y-axis: ▪ **Wavelength** ▪ To display absorbance on the y-axis, one of the following 10 options must be selected: – **Spectrum 1–Spectrum 10**

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 2nd y-axis: ▪ **Wavelength** ▪ To display absorbance on the 2nd y-axis, one of the following 10 options must be selected: – **Spectrum 1–Spectrum 10**

NOTICE

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

Execute with

For a **TEST NOISE** command to be executed, an instrument of the **2060 the NIR** type must be assigned.

See also

CAL WL – Properties (chapter 5.9.4.8, page 459)

Creating and editing a method (chapter 5.9.2.3, page 284)

TEST NOISE – Command variables (chapter 5.9.4.9.1, page 463)

TEST WL – Properties (chapter 5.9.4.10, page 463)

MEAS REF SPEC – Properties (chapter 5.9.4.7, page 457)

VAL WL – Properties (chapter 5.9.4.4, page 449)

Standards – Subsection (chapter 5.10.10, page 860)

5.9.4.9.1 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 5.9.4.9, page 461)

5.9.4.10 TEST WL – Properties

The **TEST WL** command is used to test 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.

Clicking on under **Processes ► Method ► Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **TEST WL** command:

Parameters

Measuring parameters	
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, the following specific parameter appears: – Channel
Channel	Selection of the measuring channel in which the spectra are acquired.

NOTICE

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

Execute with

For a **TEST WL** command to be executed, an instrument of the **2060 the NIR** type must be assigned.

See also

Creating and editing a method (chapter 5.9.2.3, page 284)

MEAS SPEC – Properties (chapter 5.9.4.12.7, page 502)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

5.9.4.10.1 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.

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 status of the test of the wavelength accuracy. ▪ **1**: The test was successful. ▪ **2**: The test failed.

See also

TEST WL – Properties (chapter 5.9.4.10, page 463)

5.9.4.11 EVAL BASE STATISTICS – Parameters

The **EVAL BASE STATISTICS** command is used to evaluate basic statistical results from a measuring point list. The mean value, minimum value, maximum value, integral value and standard deviation values are generated. Depending on the referenced command, the option exists of defining preprocessing measures.

NOTICE

In the method, the referenced command must be executed **before** the **EVAL BASE STATISTICS** command.

Currently, only the **MEAS SPEC** command can be referenced by the **EVAL BASE STATISTICS** command.

The **EVAL BASE STATISTICS** command is executed with the parameters listed in the following:

Referenced command	
Name of the measuring command	Selection of the command that generates the measuring point list to be evaluated. Once a measurement command has been selected, the **[Define data preprocessings]** and **[Define wavelength ranges]** buttons become visible.

Referenced command	
[Define data pre-processings]	The subsection for defining the data preprocessing is opened. More information on data preprocessing and the associated parameters: *Data preprocessing – Area (see chapter 5.11.1.11, page 890)*
[Define wave-length ranges]	The subsection for defining the wavelength ranges is opened. More information on wavelength ranges and the associated parameters: *Wavelength range – Area (see chapter 5.11.1.12, page 892)*

NOTICE

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

See also

Command – Directory (chapter 5.9.4.17, page 622)

MEAS SPEC – Properties (chapter 5.9.4.12.7, page 502)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

5.9.4.11.1 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.
'**Integral.Result**.*Command name*' Integral value of the defined wavelength range.

Command variables
'**Maximum.Result**.*Command name*'
Maximum value of the defined wavelength range.
'**Mean.Result**.*Command name*'
Mean value of the defined wavelength range.
'**Minimum.Result**.*Command name*'
Minimum value of the defined wavelength range.
'**StandardDeviation.Result**.*Command name*'
Standard deviation of the defined wavelength range.

See also

EVAL BASE STATISTICS – Parameters (chapter 5.9.4.11, page 465)

MEAS SPEC – Properties (chapter 5.9.4.12.7, page 502)

CALC – Parameters (chapter 5.9.4.16.1, page 586)

5.9.4.12 Measuring commands

5.9.4.12.1 MEAS COND – Conductivity measurement

5.9.4.12.1.1 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.

Clicking on  under **Processes ► Method ► Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.
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 as soon as the specified measured value has been reached. **Off** deactivates 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.

Measuring parameters	
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** The **Temperature coefficient** field is only displayed if **Constant factor** is selected. ▪ **DIN EN 27888** If **DIN EN 27888** is selected, only the field **Reference temperature** is displayed. This type of temperature compensation is used for the determination of ground water, spring water and surface water in accordance with DIN EN 27888. ▪ **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.

Chart – y2-axis	
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**

NOTICE

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 executed, a functional unit of the **Measuring interface conductivity** type to which a sensor of the **Conductivity measuring cell** type is connected must be assigned to the 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 5.9.4, page 293)

MEAS COND – Command variables (chapter 5.9.4.12.1.2, page 471)

MEAS CONC – Properties (chapter 5.9.4.12.6, page 495)

MEAS Ipol – Properties (chapter 5.9.4.12.4.1, page 484)

MEAS pH – Properties (chapter 5.9.4.12.2.1, page 472)

MEAS T – Properties (chapter 5.9.4.12.5, page 490)

MEAS U – Properties (chapter 5.9.4.12.3.1, page 478)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.12.1.2 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 variables available are stored in the **Command variables** variable category.

Command variables
'**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
'**Unit.Measvalue**.*Command name*' Unit of the measured values. Unit: mS/cm

See also

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

5.9.4.12.2 MEAS pH – pH measurement

5.9.4.12.2.1 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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**.
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.

Measuring parameters	
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**

NOTICE

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.

NOTICE

Further information on assigning analog sensors: *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807) Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)*

Assigning digital sensors (see chapter 5.10.5.7, page 809)

Assigning analog sensors (see chapter 5.10.5.8, page 811)

See also

Commands – Definition (chapter 5.9.4, page 293)

MEAS CONC – Properties (chapter 5.9.4.12.6, page 495)

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

MEAS Ipol – Properties (chapter 5.9.4.12.4.1, page 484)

MEAS pH – Command variables (chapter 5.9.4.12.2.2, page 477)

MEAS T – Properties (chapter 5.9.4.12.5, page 490)

MEAS U – Properties (chapter 5.9.4.12.3.1, page 478)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.12.2.2 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*' Voltage 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
'**Unit.Measvalue**.*Command name*' Unit of the measured value.

Equipment variables
'**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 5.9.4.12.2.1, page 472)

5.9.4.12.3 MEAS U – Potential measurement

5.9.4.12.3.1 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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**

NOTICE

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.

NOTICE

Further information on assigning analog sensors: *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)* *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)*

Assigning digital sensors (see chapter 5.10.5.7, page 809)

Assigning analog sensors (see chapter 5.10.5.8, page 811)

See also

Commands – Definition (chapter 5.9.4, page 293)

MEAS CONC – Properties (chapter 5.9.4.12.6, page 495)

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

MEAS Ipol – Properties (chapter 5.9.4.12.4.1, page 484)

MEAS pH – Properties (chapter 5.9.4.12.2.1, page 472)

MEAS T – Properties (chapter 5.9.4.12.5, page 490)

MEAS U – Command variables (chapter 5.9.4.12.3.2, page 483)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.12.3.2 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*' Voltage 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
'**Unit.Measvalue**.*Command name*' Unit of the measured value.

Equipment variables
'**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 5.9.4.12.3.1, page 478)

5.9.4.12.4 MEAS Ipol – Voltametric measurement

5.9.4.12.4.1 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.

Clicking on  under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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 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 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.

Measuring parameters	
Temperature	The field **Temperature** for the entry of the measuring temperature appears only if the setting **Automatic** or **Manual** has been selected.
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, we recommend entering the current in steps 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 for polarizable electrodes during the transition from an inactive normal status to the measurement. It checks within a few seconds whether an electrode is connected and that no 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**

NOTICE

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
- **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 units need to be assigned to the command.

- Analog measuring input to which the sensor required for the measurement is connected:
  Measuring Module Analog, **Measuring interface analog** or **Interface coulometry**.
- Analog sensor:
  Polarizable metal 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.
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

Commands – Definition (chapter 5.9.4, page 293)

MEAS Ipol – Command variables (chapter 5.9.4.12.4.2, page 489)

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

MEAS CONC – Properties (chapter 5.9.4.12.6, page 495)

MEAS pH – Properties (chapter 5.9.4.12.2.1, page 472)

MEAS T – Properties (chapter 5.9.4.12.5, page 490)

MEAS U – Properties (chapter 5.9.4.12.3.1, page 478)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.12.4.2 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 variables available are stored in the **Command variables** variable category.

Command variables
'**Driftvalue.Final**.*Command name*' Voltage 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
'**Unit.Measvalue**.*Command name*' Unit of the measured value.

See also

MEAS Ipol – Properties (chapter 5.9.4.12.4.1, page 484)

5.9.4.12.5 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.

Clicking on under **Processes ► Method ► Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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 activated, 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	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**.

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)

NOTICE

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 °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

For a **MEAS T** 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**, **Measuring interface analog** or **Interface coulometry**.

- Sensor (digital or analog):
  pH electrode or **Temperature 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. ▪ **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) ▪ **Pol./Temp.**: Measurement with a polarizable 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.

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.

> **NOTICE**
>
> Further information on assigning analog sensors: *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807) Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)*
>
> *Assigning digital sensors (see chapter 5.10.5.7, page 809)*
>
> *Assigning analog sensors (see chapter 5.10.5.8, page 811)*

See also

Commands – Definition (chapter 5.9.4, page 293)

MEAS CONC – Properties (chapter 5.9.4.12.6, page 495)

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

MEAS Ipol – Properties (chapter 5.9.4.12.4.1, page 484)

MEAS pH – Properties (chapter 5.9.4.12.2.1, page 472)

MEAS T – Command variables (chapter 5.9.4.12.5.1, page 494)

MEAS U – Properties (chapter 5.9.4.12.3.1, page 478)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.12.5.1 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 variables available are stored in the **Command variables** variable category.

Command variables
'**Driftvalue.Final**.*Command name*' Temperature drift (end value) after processing of the command. Unit: °C/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
'**Unit.Measvalue**.*Command name*' Unit of the measured value.

See also

MEAS T – Properties (chapter 5.9.4.12.5, page 490)

5.9.4.12.6 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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**.
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.

Measuring parameters	
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**

NOTICE

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.

NOTICE

Further information on assigning analog sensors: *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)* *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)*

Assigning digital sensors (see chapter 5.10.5.7, page 809)

Assigning analog sensors (see chapter 5.10.5.8, page 811)

See also

Commands – Definition (chapter 5.9.4, page 293)

MEAS CONC – Command variables (chapter 5.9.4.12.6.1, page 500)

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

MEAS Ipol – Properties (chapter 5.9.4.12.4.1, page 484)

MEAS pH – Properties (chapter 5.9.4.12.2.1, page 472)

MEAS T – Properties (chapter 5.9.4.12.5, page 490)

MEAS U – Properties (chapter 5.9.4.12.3.1, page 478)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.12.6.1 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*' Voltage 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
'**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
'**Slope.CurrentSensor**.*Command name*' Slope of the ion-selective electrode (ISE) used. Unit: mV
'**Unit.Blank.CurrentSensor**.*Command name*' Unit of the blank value.
'**ZeroPoint.CurrentSensor**.*Command name*' Electrode zero point E(0) of the ion-selective electrode (ISE) used. Unit: mV

See also

MEAS CONC – Properties (chapter 5.9.4.12.6, page 495)

5.9.4.12.7 MEAS SPEC – Properties

The **MEAS SPEC** command is used to acquire a spectrum of a sample. The samples are analyzed with the values **Wavelength** and **Absorbance**.

NOTICE

The **MEAS SPEC** command can be referenced in the parameters of the **PREDICT** command and the **EVAL BASE STATISTICS** command.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **MEAS SPEC** command:

Parameters

Measuring parameters	
Channel	Selection of the measuring channel in which the measured data is recorded.
Window correction	If the check box is activated, a window correction is applied when acquiring the spectrum. The window correction should be applied if the sample is placed on the reactor window. The window correction is activated by default.
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. The signal must not be saturated with an integration time that is too high.
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 takes.

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	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: ▪ **Wavelength** ▪ **Absorbance** (default value)

Curve simulation	
Curve selection	Simulated spectra from the selection list can be used to check the determination run. ▪ Deactivate the simulation by selecting **None** (default value) before analyzing real samples.

NOTICE

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

Execute with

For a **MEAS SPEC** command to be executed, an instrument of the **2060 the NIR** type must be assigned.

See also

Creating and editing a method (chapter 5.9.2.3, page 284)

MEAS SPEC – Properties (chapter 5.9.4.12.7, page 502)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

MEAS REF SPEC – Properties (chapter 5.9.4.7, page 457)

EVAL BASE STATISTICS – Parameters (chapter 5.9.4.11, page 465)

5.9.4.13 Calibration commands

5.9.4.13.1 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

When selecting a commercial buffer series, make sure that the buffer solution used is actually present in the buffer series: *Metrohm buffer type (see chapter 5.10.8.2, page 845)*
Metrohm buffer type (see chapter 5.10.8.2, page 845)

Baker buffer type (see chapter 5.10.8.3, page 846)

Beckmann buffer type (see chapter 5.10.8.4, page 847)

DIN buffer type (in accordance with DIN standard 19267, 2012) (see chapter 5.10.8.5, page 848)

Fisher buffer type (see chapter 5.10.8.6, page 849)

Fluka buffer type (see chapter 5.10.8.7, page 851)

Hamilton DURACAL buffer type (see chapter 5.10.8.8, page 852)

Merck CertiPUR 20/Titrisol buffer type (see chapter 5.10.8.9, page 853)

Buffer type Merck CertiPUR 25 (see chapter 5.10.8.10, page 854)

Mettler Toledo buffer type (see chapter 5.10.8.11, page 855)

NIST buffer type (see chapter 5.10.8.12, page 856)

Radiometer Analytical buffer type (see chapter 5.10.8.13, page 858)

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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.

Measuring parameters	
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.

Chart – y2-axis	
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**

NOTICE

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.

NOTICE

Further information on assigning analog sensors: *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)* *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)*

Assigning digital sensors (see chapter 5.10.5.7, page 809)

Assigning analog sensors (see chapter 5.10.5.8, page 811)

See also

Commands – Definition (chapter 5.9.4, page 293)

CAL pH – Calibration principle (chapter 5.9.4.13.1.1, page 509)

CAL pH – Command variables (chapter 5.9.4.13.1.2, page 511)

DET – Properties (chapter 5.9.4.2.1.2, page 299)

MEAS pH – Properties (chapter 5.9.4.12.2.1, page 472)

MET – Properties (chapter 5.9.4.2.2.2, page 324)

SET – Properties (chapter 5.9.4.2.3.2, page 348)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.13.1.1 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.

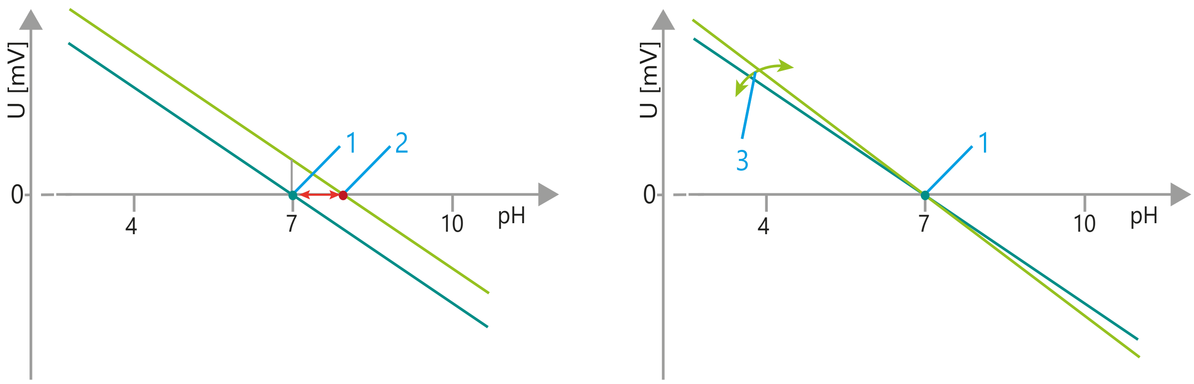


Figure 5 Deviation of the electrode zero point pH(0) and the slope from the ideal Nernst curve.

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 – Properties (chapter 5.9.4.13.1, page 504)

CAL pH – Command variables (chapter 5.9.4.13.1.2, page 511)

Editing custom calibration buffers (chapter 5.10.8.1, page 843)

5.9.4.13.1.2 CAL pH – Command variables

The following command variables are generated by the **CAL pH** command during the method run 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.

'**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

'**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

See also

CAL pH – Calibration principle (chapter 5.9.4.13.1.1, page 509)

CAL pH – Properties (chapter 5.9.4.13.1, page 504)

5.9.4.13.2 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

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.
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**

NOTICE

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.

NOTICE

Further information on assigning analog sensors: *Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807) Assigning analog sensors (Metrohm USB device) (see chapter 5.10.5.6, page 807)*

Assigning digital sensors (see chapter 5.10.5.7, page 809)

Assigning analog sensors (see chapter 5.10.5.8, page 811)

See also

Commands – Definition (chapter 5.9.4, page 293)

CAL CONC – Command variables (chapter 5.9.4.13.2.2, page 519)

CAL CONC – Calibration principle (chapter 5.9.4.13.2.1, page 517)

CAL COND – Properties (chapter 5.9.4.13.3, page 521)

CAL pH – Properties (chapter 5.9.4.13.1, page 504)

CAL WRITE – Writing calibration data (chapter 5.9.4.13.4, page 525)

Ion-selective electrode – Calibrating (chapter 5.10.5.5, page 805)

MEAS CONC – Properties (chapter 5.9.4.12.6, page 495)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.13.2.1 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.

NOTICE

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 different 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 – Properties (chapter 5.9.4.13.2, page 513)

CAL CONC – Command variables (chapter 5.9.4.13.2.2, page 519)

Ion-selective electrode – Calibrating (chapter 5.10.5.5, page 805)

5.9.4.13.2.2 CAL CONC – Command variables

The following command variables are generated by the **CAL CONC** command during the method run 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.

'**Blank.Result**.*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: Corresponds to the concentration unit, set in the variable '**Unit.Concentration.CalibrationSolution.***Command name*'

'**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: set in the variable '**Unit.Concentration.CalibrationSolution.***Command name*'

'**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

'**Unit.Concentration.CalibrationSolution.***Command name*'

Unit of the concentration of the solution that is added. It is defined by the user in the properties of the ion-selective electrode used. Unit of the concentration.

'**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

See also

CAL CONC – Properties (chapter 5.9.4.13.2, page 513)

CAL CONC – Calibration principle (chapter 5.9.4.13.2.1, page 517)

5.9.4.13.3 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **CAL COND** command:

Parameters

Conductivity standards	
Manual	Selection of the entry mode of the specifications of the conductivity standard. If **Manual** is selected, the following parameters are displayed: ▪ **Reference temperature** ▪ **Conductivity** ▪ **Temperature coefficient**
Reference temperature	Temperature at which the conductivity to be measured is known. It should be as close to the measuring temperature as possible.
Conductivity	Conductivity κ of the standard at reference temperature.
Temperature coefficient	Temperature coefficient of the standard at reference temperature.
Template	Selection of the entry mode of the specifications of the conductivity standard. If **Template** is selected, the template for the standard must be selected with the **Conductivity standard** parameter.
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**
Time-controlled measurement	Selection of the measuring mode. If **Time-controlled measurement** is selected, the following specific parameter is displayed: ▪ **Measurement duration**
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.
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 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.

Measuring parameters	
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.
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**

NOTICE

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 executed, a functional unit of the **Measuring interface conductivity** type to which a sensor of the **Conductivity measuring cell** type is connected must be assigned to the 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 5.9.4, page 293)

CAL COND – Command variables (chapter 5.9.4.13.3.1, page 524)

CAL CONC – Properties (chapter 5.9.4.13.2, page 513)

CAL pH – Properties (chapter 5.9.4.13.1, page 504)

CAL WRITE – Writing calibration data (chapter 5.9.4.13.4, page 525)

COND CHECK – Parameters (chapter 5.9.4.2.14.1, page 442)

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

Creating a Conductivity table (chapter 5.10.9, page 859)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.13.3.1 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 variables available are stored in the **Command variables** variable category.

'**CellConstant**.*Command name*'
Cell constant after processing the command.
Unit: cm^{-1}

'**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

'**Unit.Measvalue**.*Command name*'

Unit of the measured values.

Unit: mS/cm

See also

CAL COND – Properties (chapter 5.9.4.13.3, page 521)

5.9.4.13.4 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.

NOTICE

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

Command – Properties (chapter 5.9.4.1, page 295)

CAL CONC – Properties (chapter 5.9.4.13.2, page 513)

CAL COND – Properties (chapter 5.9.4.13.3, page 521)

CAL pH – Properties (chapter 5.9.4.13.1, page 504)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.14 Dosing commands

5.9.4.14.1 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.

Clicking on  under **Processes ► Method ► Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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 dosing 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, 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.

NOTICE

Further 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.

See also

Commands – Definition (chapter 5.9.4, page 293)

ADD – Command variables (chapter 5.9.4.14.2, page 528)

FILL – Properties (chapter 5.9.4.14.8, page 548)

PISTON POS – Properties (chapter 5.9.4.14.12, page 558)

PISTON END – Properties (chapter 5.9.4.14.10, page 553)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.14.2 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

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)
'**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

Equipment variables
'**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
'**Length.Tube.SpecialPort.CurrentCylinderUnit**.*Command name*' Length of the connection tubing that is connected to the special port of the cylinder unit. Unit: cm

Equipment variables
'**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.
'**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 5.9.4.14.1, page 526)

5.9.4.14.3 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.

NOTICE

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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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

Commands – Definition (chapter 5.9.4, page 293)

ASPIRATE – Command variables (chapter 5.9.4.14.4, page 535)

DOSE – Properties (chapter 5.9.4.14.6, page 542)

COMPENSATE – Properties / Execute with (chapter 5.9.4.14.5, page 538)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.14.4 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 5.9.4.14.3, page 532)

5.9.4.14.5 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.

NOTICE

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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

COMPENSATE – Command variables (chapter 5.9.4.14.5.1, page 540)

ASPIRATE – Properties (chapter 5.9.4.14.3, page 532)

DOSE – Properties (chapter 5.9.4.14.6, page 542)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.14.5.1 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

Equipment variables
'**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
'**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

Equipment variables
'**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 5.9.4.14.5, page 538)

5.9.4.14.6 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.

NOTICE

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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

DOSE – Command variables (chapter 5.9.4.14.7, page 544)

COMPENSATE – Properties / Execute with (chapter 5.9.4.14.5, page 538)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.14.7 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

Command variables
'**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.
'**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
'**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

Equipment variables
'**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
'**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

Equipment variables
'**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 5.9.4.14.6, page 542)

5.9.4.14.8 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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

Commands – Definition (chapter 5.9.4, page 293)

FILL – Command variables (chapter 5.9.4.14.9, page 550)

ADD – Properties (chapter 5.9.4.14.1, page 526)

PISTON POS – Properties (chapter 5.9.4.14.12, page 558)

PISTON END – Properties (chapter 5.9.4.14.10, page 553)

Creating and editing a method (chapter 5.9.2.3, page 284)

805 Dosimat – Properties / Specific data (chapter 5.10.2.6, page 710)
805 Dosimat – Properties / Specific data (chapter 5.10.2.6, page 710)
Dosing device (MSB) – Properties / Specific data (chapter 5.10.2.7, page 711)

Dosing unit (OMNIS) – Properties / Specific data (chapter 5.10.2.8, page 715)

5.9.4.14.9 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)
'**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

Equipment variables
'**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
'**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

Equipment variables
'**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 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 5.9.4.14.8, page 548)

5.9.4.14.10 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.

NOTICE

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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

The maximum dosing and filling rates that were defined in the Equipment are not taken into consideration for this command.

NOTICE

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

Commands – Definition (chapter 5.9.4, page 293)

PISTON END – Command variables (chapter 5.9.4.14.11, page 555)

ADD – Properties (chapter 5.9.4.14.1, page 526)

FILL – Properties (chapter 5.9.4.14.8, page 548)

PISTON POS – Properties (chapter 5.9.4.14.12, page 558)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.14.11 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)

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 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
'**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 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 5.9.4.14.10, page 553)

5.9.4.14.12 PISTON POS – Properties

The **PISTON POS** command is used to move the piston to a certain position in the dosing 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

The maximum dosing and filling rates that were defined in the Equipment are not taken into consideration for this command.

NOTICE

Further 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

Commands – Definition (chapter 5.9.4, page 293)

PISTON POS – Command variables (chapter 5.9.4.14.13, page 560)

ADD – Properties (chapter 5.9.4.14.1, page 526)

FILL – Properties (chapter 5.9.4.14.8, page 548)

PISTON END – Properties (chapter 5.9.4.14.10, page 553)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.14.13 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

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 POS – Properties (chapter 5.9.4.14.12, page 558)

5.9.4.14.14 SOLVENT HANDLING – Properties

The **SOLVENT HANDLING** command is used for conveying liquids with the OMNIS Solvent Module.

> **NOTICE**
>
> 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

> **NOTICE**
>
> 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

Command – Properties (chapter 5.9.4.1, page 295)

ADD – Properties (chapter 5.9.4.14.1, page 526)

FILL – Properties (chapter 5.9.4.14.8, page 548)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.14.15 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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 5.9.4, page 293)

PISTON POS – Properties (chapter 5.9.4.14.12, page 558)

PISTON END – Properties (chapter 5.9.4.14.10, page 553)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15 Automation commands

5.9.4.15.1 OPEN GRIPPER – Properties / Execute with

The **OPEN GRIPPER** command is used for opening the gripper fingers on the gripper arm of a sample robot

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In order for an **OPEN GRIPPER** command to be executed, a functional unit of the **Main module Pick&Place** type needs to have been assigned to it beforehand in the **Execute with** subsection.

See also

Command – Properties (chapter 5.9.4.1, page 295)

MOVE TO RACK – Properties (chapter 5.9.4.15.6, page 571)

CLOSE GRIPPER – Properties / Execute with (chapter 5.9.4.15.2, page 565)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.2 CLOSE GRIPPER – Properties / Execute with

The **CLOSE GRIPPER** command is used to close the gripper fingers on the gripper arm of the sample robot around the sample beaker so that it can be moved with a secure grip. The opening radius of the gripper fingers is determined automatically by the diameter of the sample beaker to be moved.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In order for a **CLOSE GRIPPER** command to be executed, a functional unit of the **Main module Pick&Place** type needs to have been assigned to it beforehand in the **Execute with** subsection.

See also

Command – Properties (chapter 5.9.4.1, page 295)

Creating and editing a method (chapter 5.9.2.3, page 284)

OPEN GRIPPER – Properties / Execute with (chapter 5.9.4.15.1, page 565)

5.9.4.15.3 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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 5.9.4.1, page 295)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.4 LIFT – Properties

The **LIFT** command is used to move the lifts of sample robots or sample changers to a defined lift height.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **LIFT** command:

Parameters

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 specific 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***: 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: *Defining the lift height (see chapter 5.10.2.43, page 774)*.
Lift height	Enter the height (in mm) to which the lift is 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, an error message is 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 moved. The default value **Maximum** corresponds to the maximum speed that the executing functional unit permits. ***Note***: The instrument checks during dosing that this speed does not exceed the maximum speed that the executing functional unit permits. If the **Lift rate** defined here exceeds the maximum permitted speed, an error message is displayed.

NOTICE

Further 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 instrument or functional unit used, different input ranges apply for the following parameters:

- **Lift height**
  - **Main module Pick&Place**:
    Minimum value: 0 mm
    Maximum value: 202 mm
  - **Pick&Place module**:
    Minimum value: 0 mm
    Maximum value: 130 mm
  - **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: 110 mm
- **Lift rate**
  - **OMNIS Sample Robot**:
    Minimum value: 1 mm/s
    Maximum value: 75 mm/s
  - **USB Sample Processor**:
    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**
- **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

Command – Properties (chapter 5.9.4.1, page 295)

LIFT – Command variables (chapter 5.9.4.15.4.1, page 569)

Defining the lift height (chapter 5.10.2.43, page 774)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.4.1 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 5.9.4.15.4, page 566)

5.9.4.15.5 MOVE TO EXT – Properties

The **MOVE TO EXT** command is used to move to an external position.

Clicking on [icon] under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

Command – Directory (chapter 5.9.4.17, page 622)

MOVE TO EXT – Command variables (chapter 5.9.4.15.5.1, page 570)

Creating and editing a method (chapter 5.9.2.3, page 284)

786 Swing Head – Properties (chapter 5.10.2.42, page 772)

5.9.4.15.5.1 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 5.9.4.15.5, page 569)

5.9.4.15.6 MOVE TO RACK – Properties

The **MOVE TO RACK** command is used to approach a specific position on the sample rack or the park position.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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***Editing subsample data (see chapter 5.9.1.8.1, page 275)*. 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** type: – **'Rack name'**: Name of the sample rack – **PARK**: Park position – **RP1–RP7**: Absolute rack position Instruments of the **USB Sample Processor** type: – Metrohm recommends entering the order number so that the rack used can be identified unambiguously (8-digit number, e.g. 62041720). – **PARK**: Park position
Position on the rack	Select a 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***Editing subsample data (see chapter 5.9.1.8.1, page 275)*. 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 special position. If **Special position** is selected, the following specific parameter appears: – **Index** ▪ **Enter position**: Entry of an absolute position on the sample rack. If **Enter position** is selected, 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***Defining a special position (see chapter 5.10.2.44, page 778)*.
Target position	Enter the position on the selected sample rack. The position numbers are marked on the sample rack. The number of positions on the rack depends on the respective sample rack.

Execute with

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**
- **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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

MOVE TO RACK – Command variables (chapter 5.9.4.15.6.1, page 573)

Creating and editing a method (chapter 5.9.2.3, page 284)

Defining a special position (chapter 5.10.2.44, page 778)

5.9.4.15.6.1 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.

Command variables
'**Sampleposition.Final**.*Command name*' **OMNIS Sample Robot**: 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 approached by the gripper arm is or the park position (**PARK**). **USB Sample Processor**: Designation of the rack (e.g. **order number**) on which the approached position is or the park position (**PARK**).

See also

MOVE TO RACK – Properties (chapter 5.9.4.15.6, page 571)

5.9.4.15.7 MOVE TO WORKSTATION – Properties / Execute with

The **MOVE TO WORKSTATION** command is used to move the gripper arm to the required workstation and position the gripper above the target position.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In order for a **MOVE TO WORKSTATION** command to be executed, a functional unit of the **Main module Pick&Place** type and a functional unit of the **Pick&Place module** type need to have been assigned to it beforehand in the **Execute with** subsection.

See also

Command – Properties (chapter 5.9.4.1, page 295)

MOVE TO WORKSTATION – Command variables (chapter 5.9.4.15.7.1, page 574)

MOVE TO RACK – Properties (chapter 5.9.4.15.6, page 571)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.7.1 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 variable available is 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.
'**Targetposition.Final**.*Command name'* Workstation that was approached with the command. The workstation number **WM2**, **WM3**, **WM5** or **WM6** is output as the variable content. Workstations **WM1** and **WM4** are reserved for pump modules, meaning that they cannot be approached to process samples.

Arrangement of the workstation

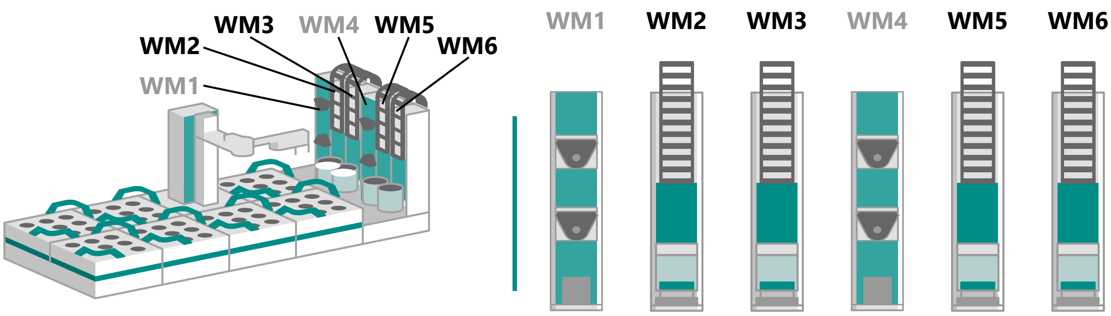


Figure 6 Sample design of a module OMNIS Sample Robot.

See also

MOVE TO WORKSTATION – Properties / Execute with (chapter 5.9.4.15.7, page 574)

5.9.4.15.8 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**.

NOTICE

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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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

Commands – Definition (chapter 5.9.4, page 293)

ADD – Properties (chapter 5.9.4.14.1, page 526)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.9 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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

Commands – Definition (chapter 5.9.4, page 293)

Command – Directory (chapter 5.9.4.17, page 622)

ROTATE ANGLE – Command variables (chapter 5.9.4.15.9.1, page 577)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.9.1 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: °
'**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 5.9.4.15.9, page 577)

5.9.4.15.10 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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 5.9.4.1, page 295)

LIFT – Properties (chapter 5.9.4.15.4, page 566)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.11 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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 5.9.4, page 293)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.12 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

Command – Directory (chapter 5.9.4.17, page 622)

SWING ANGLE – Command variables (chapter 5.9.4.15.12.1, page 581)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.12.1 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: °

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

SWING ANGLE – Properties (chapter 5.9.4.15.12, page 580)

5.9.4.15.13 PARK LID – Properties / Execute with

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.

NOTICE

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.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In order for a **PARK LID** command to be executed, a functional unit of the **Main module Pick&Place** type needs to have been assigned to it beforehand in the **Execute with** subsection.

See also

Command – Properties (chapter 5.9.4.1, page 295)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.14 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.

NOTICE

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.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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.

NOTICE

The lift height of the sample beaker must be specified. The OMNIS Software takes the thickness of the lid automatically into account.

NOTICE

Further 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** type and a functional unit of the **Pick&Place module** type need to have been assigned to the command.

See also

Command – Properties (chapter 5.9.4.1, page 295)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.15.15 FLOW – Properties

The **FLOW** command is used for setting the carrier gas flow of the gas flow module.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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, 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 selection) 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 selection) ▪ **Nitrogen**

NOTICE

Further 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 module** type needs to be assigned to the command.

See also

Command – Properties (chapter 5.9.4.1, page 295)

Gas flow module – Manual control (chapter 5.10.2.20, page 750)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Creating and editing a method (chapter 5.9.2.3, page 284)

TEMP – Properties (chapter 5.9.4.15.16, page 585)

5.9.4.15.16 TEMP – Properties

The **TEMP** command is used for setting the temperature of the oven module. A **TEMP** can be skipped during the run with a **SKIP** command or in the **Live data**. In this case, the command will be ended but the temperature control continues to run.

NOTICE

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.

Clicking on under **Processes ▶ Method ▶ Command** opens the **Properties** window. In the **General** subsection, the name and object ID are displayed: *Command – Properties (see chapter 5.9.4.1, page 295)*. In the 2 subsections **Parameters** and **Execute with**, the following functions and information are available for the **TEMP** command:

Parameters

Oven	Switch the oven on or off. If **On** is selected, the following specific parameters are displayed: ▪ **Temperature control** ▪ **Target temperature** If **Off** is selected, no further parameters are displayed.
Temperature control	Selection of the type of temperature control: ▪ **Fixed target temperature** The target temperature is reached as quickly as possible. ▪ **Gradient** The target temperature is reached with the predefined gradient.
Target temperature	Temperature to which the oven is to be set. Depending on the temperature entered, the oven can be heated or cooled. The permissible temperature range for the **874 Oven Sample Processor** lies between 50 and 250 °C.

Temperature gradient	The parameter **Temperature gradient** is only displayed if **Gradient** is selected. Gradient for the oven heating. Starting with the current oven temperature, the target temperature is to be reached with the defined temperature gradient.

NOTICE

Further 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 module** type needs to be assigned to the command.

See also

Commands – Definition (chapter 5.9.4, page 293)

FLOW – Properties (chapter 5.9.4.15.15, page 584)

Karl Fischer titration coulometric – Properties (chapter 5.9.4.2.10.1, page 422)

Creating and editing a method (chapter 5.9.2.3, page 284)

Oven module – Manual control (chapter 5.10.2.19, page 749)

5.9.4.16 Additional commands

5.9.4.16.1 CALC – Parameters

The **CALC** command is used for calculating results. The required formula can be created using the formula editor.

NOTICE

Only one result can be calculated per **CALC** command. If several results should be calculated, then several commands have to be added.

NOTICE

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 fx 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.

NOTICE

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

See also

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Command – Properties (chapter 5.9.4.1, page 295)

CALC – Command variables (chapter 5.9.4.16.1.1, page 588)

Formula editor – Brief description (chapter 5.9.5, page 637)

Creating and editing a method (chapter 5.9.2.3, page 284)

NOTIFY – Parameters (chapter 5.9.4.16.7, page 599)

Result monitoring – Definition (chapter 5.9.1.9, page 278)

REQUEST – Parameters (chapter 5.9.4.16.12, page 609)

Editing subsample data (chapter 5.9.1.8.1, page 275)

Reprocessing subsample data (chapter 5.8.5.4, page 188)

Monitoring – Definition (chapter 5.8.22, page 251)

5.9.4.16.1.1 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 5.9.4.16.1, page 586)

Formula editor – Brief description (chapter 5.9.5, page 637)

NOTIFY – Parameters (chapter 5.9.4.16.7, page 599)

5.9.4.16.2 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.

NOTICE

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 5.9.4.1, page 295)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Karl Fischer titration – Principle (chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (chapter 5.9.4.2.9.2, page 402)

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

KFT – Command variables (chapter 5.9.4.2.9.5, page 418)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.3 EVAL LINEAR REGRESSION – Parameters

The **EVAL LINEAR REGRESSION** command is used to carry out a linear regression with the data points of a measuring point list. The measuring points of a specific measured quantity are averaged within a defined evaluation window.

The following values are output under **Sample list ► Results ► Raw data** and in the report:

- Slope
- y-intercept
- Coefficient of determination R^2
- Number of data points
- 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

NOTICE

In the method, the referenced command must be executed **before** the **EVAL BASE STATISTICS** command. This command generates the measured values for the regression analysis. Only measured values that are valid and lie within the defined evaluation window are included. At least 2 valid measured values must be found in the evaluation window to successfully carry out the linear regression.

Currently, only the **STAT pH** command or the **STAT U** command can be referenced by the **EVAL LINEAR REGRESSION** command.

The **EVAL LINEAR REGRESSION** command is executed with the parameters listed in the following:

Name of the measuring command	Selection of the command that generates the measuring point list to be evaluated.
Quantity on the x-axis	Independent variable that is to be shown on the x-axis at the time of the evaluation: ▪ **Time** ▪ **Volume**
Lower limit	Defines the lower limit of the evaluation window. The value of the lower limit is contained in the evaluation window.
Upper limit	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	Dependent variable that is to be shown on the y-axis at the time of the evaluation: ▪ **Time** ▪ **Volume** ▪ **Drift** ▪ **Temperature** Only valid for **STAT pH**: ▪ **pH** Only valid for **STAT U**: ▪ **Potential**

NOTICE

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

See also

Command – Directory (chapter 5.9.4.17, page 622)

EVAL LINEAR REGRESSION – Command variables (chapter 5.9.4.16.3.1, page 592)

STAT – Principle (chapter 5.9.4.2.4, page 369)

5.9.4.16.3.1 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.
'**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.

Command variables
'**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.Slope.Result**.*Command name*'
Standard error of slope.
'**StandardError.Intercept.Result**.*Command name*'
Standard error of y-intercept.
'**StandardError.YEstimate.Result**.*Command name*'
Standard error of estimate y.

See also

CALC – Parameters (chapter 5.9.4.16.1, page 586)

5.9.4.16.4 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: >, <, :, ", /, \, |, *, ?, 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**).

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

Operating procedure – Properties (chapter 5.9.1.2, page 262)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.5 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 fx 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.

NOTICE

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

See also

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Command – Properties (chapter 5.9.4.1, page 295)

IF – Concept (chapter 5.9.4.16.5.1, page 596)

Creating and editing a method (chapter 5.9.2.3, page 284)

NOTIFY – Parameters (chapter 5.9.4.16.7, page 599)

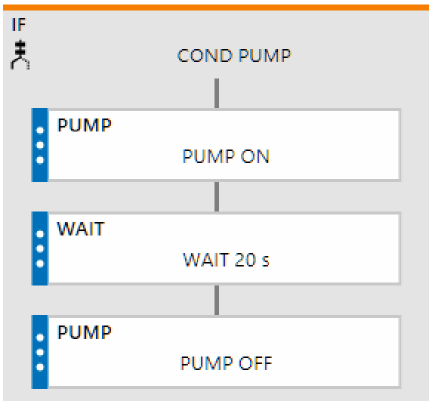
5.9.4.16.5.1 IF – Concept

Structure

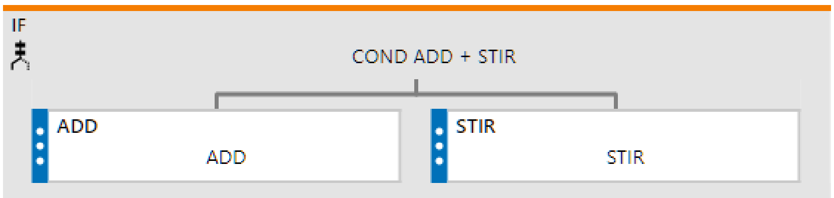
The **IF** command can be used to define a run of commands and methods that are then carried out only if the condition defined in the **IF** command is met.

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

IF – Parameters (chapter 5.9.4.16.5, page 595)

Creating and editing a method (chapter 5.9.2.3, page 284)

NOTIFY – Parameters (chapter 5.9.4.16.7, page 599)

5.9.4.16.6 LOOP – Parameters

The **LOOP** command is used to create a sequence of commands and methods which can be repeated multiple times.

The **LOOP** command is executed with the following parameters:

Number of runs	Information regarding how often the command sequence defined in the command is carried out (number of iterations). If a formula is defined for the **Number of runs** parameter and an error occurs when calculating the formula, the **LOOP** command is skipped and the process sequence is continued.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

LOOP – Concept (chapter 5.9.4.16.6.1, page 597)

LOOP – Command variables (chapter 5.9.4.16.6.2, page 598)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

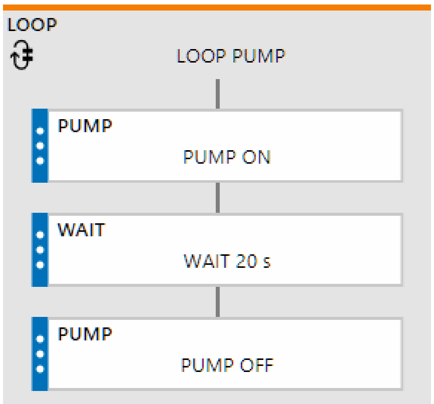
5.9.4.16.6.1 LOOP – Concept

Structure

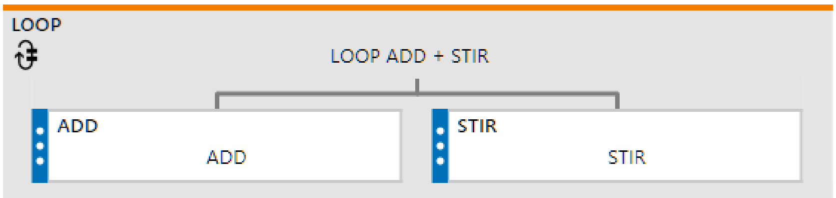
The **LOOP** command can be used to define a sequence of commands and methods that can be carried out several times.

In these sequences, serial and parallel process sequences are displayed as follows:

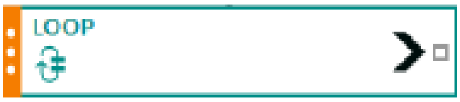
- **Serial sequence**



- **Parallel sequence**



Representation in operating procedures and methods



Clicking on ❯ shows the sequence 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 LOOP sequence does not contain any commands.

❮■ The LOOP sequence contains commands.

See also

LOOP – Parameters (chapter 5.9.4.16.6, page 597)

LOOP – Command variables (chapter 5.9.4.16.6.2, page 598)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.6.2 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.

'**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.

'**LoopCount**.*Command name*'

Number of iterations of the **LOOP** command that have been run.

Unit: None

See also

LOOP – Concept (chapter 5.9.4.16.6.1, page 597)

LOOP – Parameters (chapter 5.9.4.16.6, page 597)

5.9.4.16.7 NOTIFY – Parameters

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.

NOTICE

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: *Setting up notifications (see chapter 5.13.2, page 932)*

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.

NOTICE

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

Run in case of a limit value violation – Definition (chapter 5.9.3.3, page 293)

Setting up notifications (chapter 5.13.2, page 932)

Command – Properties (chapter 5.9.4.1, page 295)

IF – Parameters (chapter 5.9.4.16.5, page 595)

Result monitoring – Definition (chapter 5.9.1.9, page 278)

Recording the result monitoring (chapter 5.9.1.9.1, page 278)

Text editor – Brief description (chapter 5.9.6, page 657)

5.9.4.16.8 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.

NOTICE

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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

READ – Command variables (chapter 5.9.4.16.8.2, page 603)

WEIGH – Parameters (chapter 5.9.4.16.21, page 620)

WRITE – Parameters (chapter 5.9.4.16.23, page 621)

TARE – Parameters (chapter 5.9.4.16.17, page 615)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.8.1 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.

NOTICE

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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

READ – Command variables (chapter 5.9.4.16.8.2, page 603)

WEIGH – Parameters (chapter 5.9.4.16.21, page 620)

WRITE – Parameters (chapter 5.9.4.16.23, page 621)

TARE – Parameters (chapter 5.9.4.16.17, page 615)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.8.2 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 5.9.4.16.8, page 601)

5.9.4.16.9 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.

NOTICE

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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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

Remote Box MSB – Properties (chapter 5.10.2.39, page 765)

Command – Properties (chapter 5.9.4.1, page 295)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.10 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.

> **NOTICE**
>
> 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: *Command – Properties (see chapter 5.9.4.1, page 295)*. 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

Remote Box MSB – Properties (chapter 5.10.2.39, page 765)

Command – Properties (chapter 5.9.4.1, page 295)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.11 REPORT – Parameters

The **REPORT** command is used to create a report as a PDF file or to print it directly on a printer.

NOTICE

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.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Operating procedure – Properties (chapter 5.9.1.2, page 262)

Creating and editing a method (chapter 5.9.2.3, page 284)

Setting up OMNIS Software (chapter 4.3, page 17)

Setting up a printer (chapter 5.13.1, page 932)

5.9.4.16.12 REQUEST – Parameters

The **REQUEST** command is used to request subsample data or variables during determination.

The determination can be held 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 over the status menu.

[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**.
Display pop-up window	When activating the **Display pop-up window** check box, a pop-up window for data request will be displayed. Data can still be entered under **Samples ▶ Sample lists ▶ Curves and data ▶ Live data**. The command is completed with **[Continue]** or with the key combination **[CTRL]**+**[Enter]**. If the check box **Close pop-up window automatically** is activated in the window for data request, the request is automatically closed as soon as an external instrument (e.g. a balance) receives the CR/LF character string.
Name	Designation of the variable. The variable name is displayed under **Samples ▶ Sample lists ▶ Curves and data ▶ Live data**.

Variable

The data requested during the run is saved in the selected, existing variable. If the **Variable** option was selected, then the following parameters are available:

Use as	The following options are available for selection: ▪ **Input field:** The data can be modified manually. ▪ **Sample size:** Weight and weight unit 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 run is saved. Clicking *(x)* opens a dialog window 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	Activate this check box if the unit for the variable is edited during the determination.

User-defined variable

The data requested during the run 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 the **User-defined variable** option was selected, then the following parameters are available:

Use as	The following options are available for selection: ▪ **Input field:** The data can be modified manually. ▪ **Sample size:** Weight and weight unit can be applied directly in the **REQUEST** command and can be changed manually after data transmission.
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.
Edit unit	Activate this check box if the unit for the variable is edited during the determination.
Default unit	A default unit can be specified for the unit of the variable. If the **Edit unit** check box is activated, the unit for the variable can be edited.

NOTICE

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

See also

Commands – Definition (chapter 5.9.4, page 293)

Creating and editing a method (chapter 5.9.2.3, page 284)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

REQUEST – Command variables (chapter 5.9.4.16.12.1, page 611)

Carrying over weighing data to subsamples (chapter 5.8.5.3, page 186)

READ – Parameters (chapter 5.9.4.16.8, page 601)

CALC – Parameters (chapter 5.9.4.16.1, page 586)

WEIGH – Parameters (chapter 5.9.4.16.21, page 620)

WRITE – Parameters (chapter 5.9.4.16.23, page 621)

TARE – Parameters (chapter 5.9.4.16.17, page 615)

Text editor – Brief description (chapter 5.9.6, page 657)

Input field – Brief description (chapter 5.9.5.1, page 639)

5.9.4.16.12.1 REQUEST – Command variables

The following variable is created in the process sequence by the **REQUEST** command if data is requested with a **User-defined variable** 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.

'**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 5.9.4.16.12, page 609)

5.9.4.16.13 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 5.9.4.1, page 295)

SEQUENCE – Concept (chapter 5.9.4.16.13.1, page 612)

Creating and editing a method (chapter 5.9.2.3, page 284)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

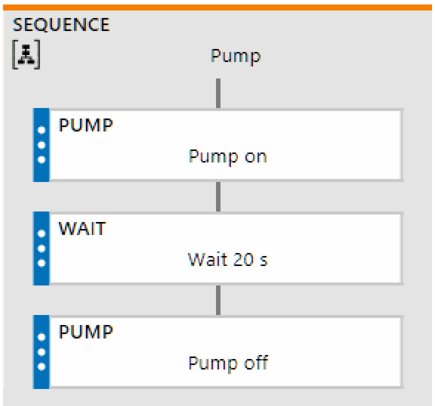
5.9.4.16.13.1 SEQUENCE – Concept

Structure

With the **SEQUENCE** command, a subordinate run sequence can be defined for commands and methods.

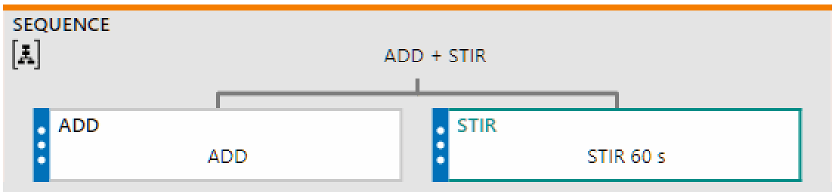
In these run sequences, serial and parallel process sequences are displayed as follows:

- **Serial sequence**



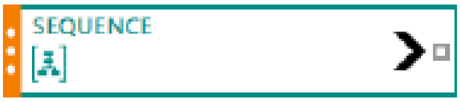
The commands within the run sequence are executed consecutively. The run sequence is concluded as soon as the last command has been completed.

- **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

SEQUENCE – Executing a sequence (chapter 5.9.4.16.13, page 612)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.14 SKIP – Parameters

The **SKIP** command is used to stop a selected command automatically. The **SKIP** command can end commands within the same operating procedure.

> **NOTICE**
>
> 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 5.9.4.1, page 295)

Creating and editing a method (chapter 5.9.2.3, page 284)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Displaying live data and controlling run (chapter 5.8.9, page 222)

5.9.4.16.15 STOP – Parameters

The **STOP** command is used to stop a determination.

The **STOP** command is executed with the following parameters:

STOP options	▪ **Stop running subsample** The determination of the current subsample is stopped. If a series determination is executed, the determination of the next subsample is not started. ▪ **Stop running series** The determination of the current subsample is stopped. The determination of the next subsample is **not** started. ▪ **Stop after running subsample** The determination is stopped after the run of the current subsample is completed.

NOTICE

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

See also

Commands – Definition (chapter 5.9.4, page 293)

Creating and editing a method (chapter 5.9.2.3, page 284)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

5.9.4.16.16 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 fx 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**.

NOTICE

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

See also

Commands – Definition (chapter 5.9.4, page 293)

Creating and editing a method (chapter 5.9.2.3, page 284)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

5.9.4.16.17 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.

NOTICE

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

See also

Commands – Definition (chapter 5.9.4, page 293)

READ – Parameters (chapter 5.9.4.16.8, page 601)

WRITE – Parameters (chapter 5.9.4.16.23, page 621)

WEIGH – Parameters (chapter 5.9.4.16.21, page 620)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.18 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 subsamples 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**.

NOTICE

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.

NOTICE

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**, **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 5.9.4.1, page 295)

Creating and editing a method (chapter 5.9.2.3, page 284)

Saving titer (chapter 5.9.4.16.19, page 618)

5.9.4.16.19 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.

> **NOTICE**
>
> 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**.
>
> *Recording the result monitoring (see chapter 5.9.1.9.1, page 278)*

See also

TITER WRITE – Parameters (chapter 5.9.4.16.18, page 616)

TITER WRITE – Parameters (chapter 5.9.4.16.18, page 616)

Recording the result monitoring (chapter 5.9.1.9.1, page 278)

5.9.4.16.20 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**.

> **NOTICE**
>
> 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**.

NOTICE

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

See also

Command – Properties (chapter 5.9.4.1, page 295)

Creating and editing a method (chapter 5.9.2.3, page 284)

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Text editor – Brief description (chapter 5.9.6, page 657)

5.9.4.16.21 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.

NOTICE

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

See also

Commands – Definition (chapter 5.9.4, page 293)

WEIGH – Command variables (chapter 5.9.4.16.22, page 621)

READ – Parameters (chapter 5.9.4.16.8, page 601)

WRITE – Parameters (chapter 5.9.4.16.23, page 621)

TARE – Parameters (chapter 5.9.4.16.17, page 615)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.16.22 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 5.9.4.16.21, page 620)

5.9.4.16.23 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 following parameters:

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

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

See also

Commands – Definition (chapter 5.9.4, page 293)

READ – Parameters (chapter 5.9.4.16.8, page 601)

WEIGH – Parameters (chapter 5.9.4.16.21, page 620)

TARE – Parameters (chapter 5.9.4.16.17, page 615)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.9.4.17 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
FLOW	Gas flow module	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
	Tower	814 USB Sample Processor, 815 Robotic USB Sample Processor XL, 855 Robotic Titrosampler, 874 Oven Sample Processor

Automation command	Functional unit	Instrument
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
	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
OPEN GRIPPER	Main module Pick&Place	OMNIS Sample Robot
PARK LID	Main module Pick&Place	OMNIS Sample Robot
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 Sample Robot
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 Dosing Module, OMNIS Sample Robot, 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 module	874 Oven Sample Processor

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 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	2060 the NIR
CAL WRITE	–	–
REF STD	2060 the NIR	2060 the NIR
TITER WRITE	–	–

Calibration command	Functional unit	Instrument
VAL REF STD	2060 the NIR	2060 the NIR
VAL WL	2060 the NIR	2060 the NIR

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 interface conductivity	856 Conductivity Module
MEAS Ipol	Measuring Module Analog	OMNIS Titrator, OMNIS Titration 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	2060 the NIR
MEAS SPEC	2060 the NIR	2060 the NIR
MEAS T	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	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

Measuring command	Functional unit	Instrument
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
EVAL BASE STATISTICS	–	–
PREDICT	–	–
TEST NOISE	2060 the NIR	2060 the NIR
TEST WL	2060 the NIR	2060 the NIR

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

Titration command	Functional unit	Instrument
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
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	Interface coulometry	851 Titrando, 852 Titrando

Titration command	Functional unit	Instrument
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 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
	Interface coulometry	852 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

Titration command	Functional unit	Instrument
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
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

Titration command	Functional unit	Instrument
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
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

Titration command	Functional unit	Instrument
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
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

Titration command	Functional unit	Instrument
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
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

Conditioning command	Functional unit	Instrument
COND CHECK	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, 890 Titrando, 901 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Interface coulometry	851 Titrando, 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, 890 Titrando, 904 Titrando, 906 Titrando
COND OFF	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, 890 Titrando, 901 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Interface coulometry	851 Titrando, 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, 890 Titrando, 904 Titrando, 906 Titrando

Conditioning command	Functional unit	Instrument
COND ON	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, 890 Titrando, 901 Titrando, 904 Titrando, 905 Titrando, 906 Titrando, 907 Titrando
	Interface coulometry	851 Titrando, 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, 890 Titrando, 904 Titrando, 906 Titrando

Additional commands	Functional unit	Instrument
CALC	–	–
COLLECT	–	–
CONSUME SUBSAMPLE	–	–
EVAL LINEAR REGRESSION	–	–
EXPORT	–	–
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

Additional commands	Functional unit	Instrument
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	
WAIT	–	–
WEIGH	Balance, Cubis II balance	
WRITE	Serial device	–

See also

Instruments – Directory (chapter 5.10.1.1, page 660)

Functional unit – Directory (chapter 5.10.2.1, page 697)

Creating and editing a method (chapter 5.9.2.3, page 284)

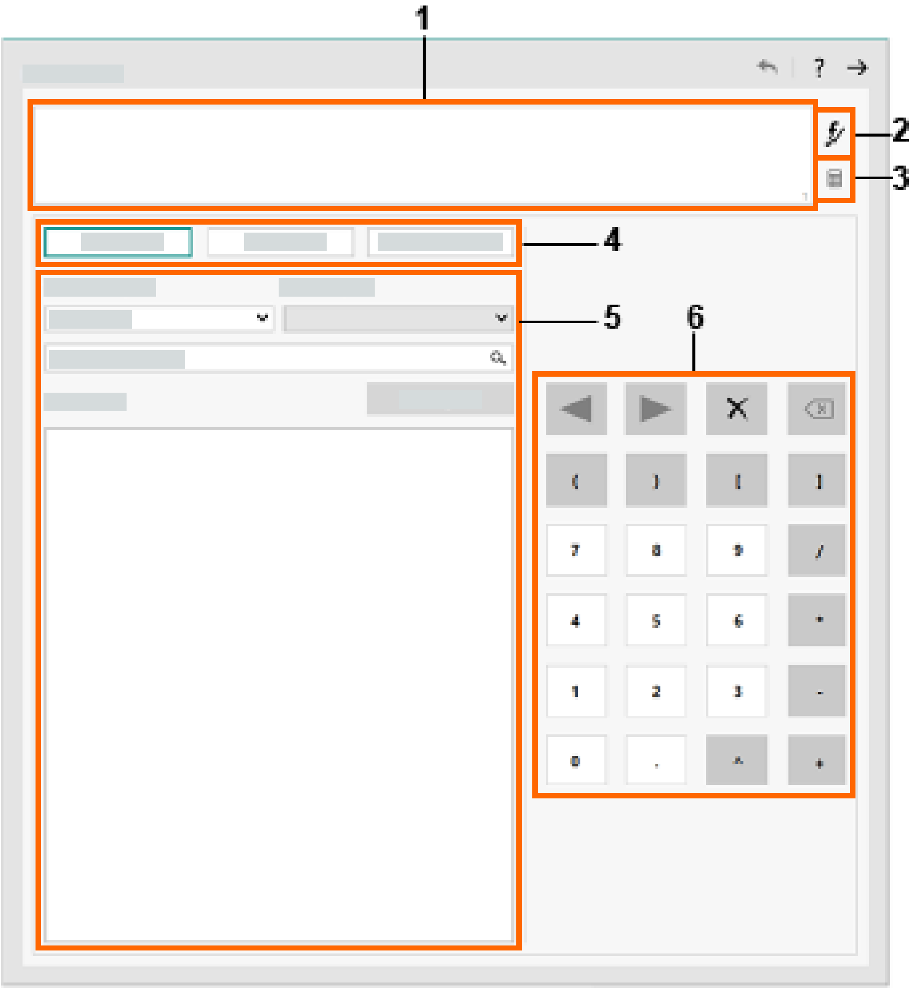
Creating a work system (chapter 5.10.3.2, page 785)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

5.9.5 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

Input field – Brief description (chapter 5.9.5.1, page 639)

Variables – Directory (chapter 5.9.5.3, page 640)

Operators – Directory (chapter 5.9.5.4, page 642)

Functions – Directory (chapter 5.9.5.5, page 644)

5.9.5.1 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]**.

5.9.5.2 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.

5.9.5.3 Variables – Directory

Variables are created automatically by the 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.

NOTICE

The variables must be inserted again in the formula editor, if a method is renamed for which variables are used to define a condition in the **IF** command.

Variable category	Subcategory	Variable type
Sample data	Selection of the sample profile.	Variables which 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.
Subsample data	Selection of the operating procedure.	Variables which 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: ▪ Creation date of the subsample: '**CreationTimestamp.CurrentSubsample**' ▪ Determination run (single determination, series determination, parallel determination): '**ExecutionMode.CurrentSubsample**'
Method variables	Selection of the method.	Variables that can be 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. **Attention:** The variables must be inserted again in the formula editor, if a method is renamed for which variables are used in the **IF** command.
Command variables	No selection.	Variables that are generated by the individual commands in the process sequence. The selection 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*'

Variable category	Subcategory	Variable type
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.

NOTICE

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.

5.9.5.4 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

NOTICE

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

NOTICE

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

NOTICE

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).

5.9.5.5 Functions – Directory

The following functions can be used in the formula editor:

Arithmetic

- **Abs** – Absolute value
  Abs – Absolute value (see chapter 5.9.5.5.1, page 645)
- **Log** – Common logarithm
  Log – Common logarithm (see chapter 5.9.5.5.2, page 646)
- **Ln** – Natural logarithm
  Ln – Natural logarithm (see chapter 5.9.5.5.3, page 646)
- **Exp** – Exponential function
  Exp – Exponential function (see chapter 5.9.5.5.4, page 647)
- **Round** – Round
  Round – Rounding (see chapter 5.9.5.5.5, page 647)
- **Sqrt** – Square root
  Sqrt – Square root (see chapter 5.9.5.5.6, page 648)

Date/Time

- **Time** – Time
  Time – Time (see chapter 5.9.5.5.7, page 648)

Type conversion

- **TextToNumber** – Convert text to number
  TextToNumber – Convert text to number (see chapter 5.9.5.5.8, page 649)
- **NumberToText** – Convert number to text
  NumberToText – Convert number to text (see chapter 5.9.5.5.9, page 649)

Text

- **TextPosition** – Return position of character string searched for
  TextPosition – Return position of character string searched for (see chapter 5.9.5.5.10, page 650)
- **Trim** – Remove blank spaces / character string
  Trim – Remove blank spaces / character string (see chapter 5.9.5.5.11, page 650)
- **SubText** – Return part of a character string
  SubText – Return part of a character string (see chapter 5.9.5.5.12, page 651)
- **Concat** – Concatenate
  Concat - Concatenating texts (see chapter 5.9.5.5.13, page 651)

Miscellaneous

- **Min** – Minimum
  Min – Minimum (see chapter 5.9.5.5.14, page 652)
- **Max** – Maximum
  Max – Maximum (see chapter 5.9.5.5.15, page 652)
- **Rand** – Generate random number
  Rand – Generate random number (see chapter 5.9.5.5.16, page 653)
- **Case** – Condition
  Case – Condition (see chapter 5.9.5.5.17, page 654)
- **Error** – Error case
  Error – Error case (see chapter 5.9.5.5.18, page 654)
- **RegEx** – Regular expression
  RegEx – Regular expression (see chapter 5.9.5.5.19, page 655)

5.9.5.5.1 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.

5.9.5.5.2 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*'.

5.9.5.5.3 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.

5.9.5.5.4 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.

5.9.5.5.5 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.

NOTICE

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 5.9.5.5, page 644)

5.9.5.5.6 Sqrt – Square root

Syntax

y = Sqrt(number)

Returns the square root of the entered number. Alternative notation for y = √ **number** or y = ^{2}√ **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*'.

5.9.5.5.7 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

5.9.5.5.8 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

5.9.5.5.9 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"

5.9.5.5.10 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.

5.9.5.5.11 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

5.9.5.5.12 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

5.9.5.5.13 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.

5.9.5.5.14 Min – Minimum

Syntax

y = Min(Number1;Number2)

Returns the smaller element (Minimum) of the two values **Number1** and **Number2**.

> **NOTICE**
>
> 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

5.9.5.5.15 Max – Maximum

Syntax

y = Max(Number1;Number2)

Returns the larger element (Maximum) of the two values **Number1** and **Number2**.

NOTICE

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

5.9.5.5.16 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.

NOTICE

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

5.9.5.5.17 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.

5.9.5.5.18 Error – Error case

Syntax

y = Error(value)

Returns **1** if the **value is invalid** (error) or **0** if the **value is valid**. This function can be used, e.g., to check variables for their existence or validity.

Parameter

Value

The variable to be tested or the value to be tested.

Examples

- Error('Result 1.*Command name*') = 0: The result could be calculated.
- Error('Result 1.*Command name*') = 1: The result could not be calculated.
- Error('Meas.EP(3).*Command name*') = 0: The variable for the measured value at endpoint 3 exists.
- Error('Meas.EP(3).*Command name*') = 1: No variable for the measured value or no EP exists.

5.9.5.5.19 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.

NOTICE

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.

5.9.6 Text editor – Brief description

The text editor is used for the entry and formatting of message texts and notifications. Graphics can also be added.

NOTICE

If text is entered, the amount must not exceed 10 A4 pages.

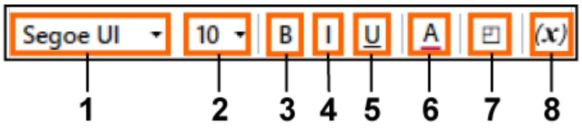
Commands

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 5.9.4.16.7, page 599)

REQUEST – Parameters (chapter 5.9.4.16.12, page 609)

WAIT – Parameters (chapter 5.9.4.16.20, page 619)

5.10 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

Instruments – Definition (chapter 5.10.1, page 660)

Work system – Definition (chapter 5.10.3, page 783)

Sensor – Definition (chapter 5.10.5, page 794)

Solution – Definition (chapter 5.10.6, page 818)

Sample rack – Definition (chapter 5.10.7, page 830)

Calibration buffers – Definition (chapter 5.10.8, page 842)

Standards – Subsection (chapter 5.10.10, page 860)

5.10.1 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

Instruments – Directory (chapter 5.10.1.1, page 660)

Reserving instruments (chapter 5.10.1.3, page 666)

Releasing instruments (chapter 5.10.1.4, page 667)

Instruments – Status (chapter 5.10.1.2, page 665)

OMNIS Software – Inventory (chapter 5.2.2, page 99)

Instruments – Manual control (chapter 5.10.1.6, page 669)

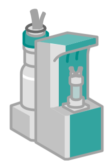
Instruments – Properties (chapter 5.10.1.5, page 668)

Backing up instrument data (chapter 5.10.1.7, page 670)

5.10.1.1 Instruments – Directory

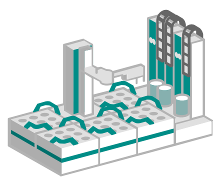
- *OMNIS instruments*
- *Metrohm USB devices*
- *Other instruments*

OMNIS instruments



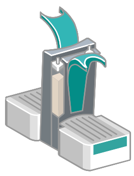
OMNIS Dosing Module

The dosing module can be used for dosing solutions. It can only be used in combination with an **OMNIS Titrator** or an **OMNIS Sample Robot** and is an extension of the **titration system** as an additional dosing unit.



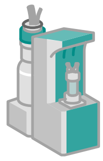
OMNIS Sample Robot

The sample robot can be used for automatic sample processing in titrations and measurements.



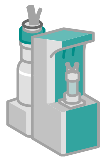
OMNIS Solvent Module

The solvent module can be used in combination with an **OMNIS Titrator** in stand-alone operation or in an automated analysis system for liquid handling tasks.



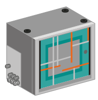
OMNIS Titration Module

The titration module can be used for automated sample analysis. It can only be used in combination with an **OMNIS Titrator** and is an extension of the **titration system** as an additional dosing unit with up to 2 measuring inputs.



OMNIS Titrator

The titrator can be used for equivalence point titrations, endpoint titrations, volumetric Karl Fischer titrations as well as concentration, pH value, potential and temperature measurements.



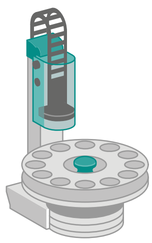
2060 the NIR

The spectrometer can be used for near-infrared spectroscopic analysis in a process environment.

Metrohm USB devices

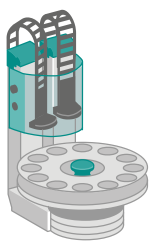
NOTICE

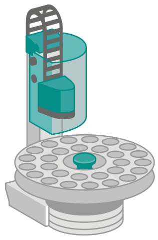
Metrohm USB devices must be connected to the same computer as the one on which the OMNIS Software is installed.

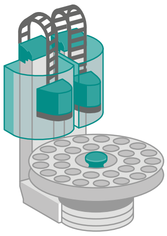


814 USB Sample Processor

The sample changer can be used for automated sample processing of titrations and measurements.

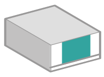






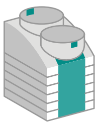
815 Robotic USB Sample Processor XL

The sample changer can be used for automated sample processing of titrations and measurements.



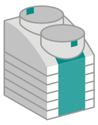
846 Dosing Interface

The dosing interface is used as interface for multiple functional units of the types MSB dosing device, MSB stirrer or Remote Box MSB and can be used for dosing auxiliary solutions.



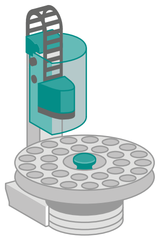
851 Titrando

The titrator can be used for coulometric Karl Fischer titrations and potential and temperature measurements.



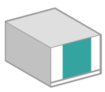
852 Titrando

The titrator can be used for volumetric and coulometric Karl Fischer titrations as well as potential and temperature measurements.



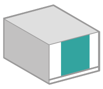
855 Robotic Titrosampler

The sample changer with integrated titrator can be used for automated sample processing as well as for equivalence point titrations, endpoint titrations and the measurement of concentration, pH value, potential and temperature.



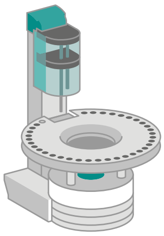
856 Conductivity Module

The conductivity measuring module can be used for conductivity measurements and for calibrating conductivity measuring cells.



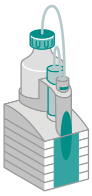
867 pH Module

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.



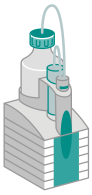
874 Oven Sample Processor

The sample changer can be used for automated thermal water extraction in Karl Fischer titrations.



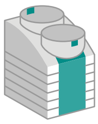
888 Titrando

The titrator can be used for volumetric Karl Fischer titrations, potentiometric titrations as well as pH value, potential and temperature measurements.



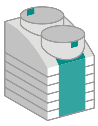
890 Titrando

The titrator can be used for volumetric Karl Fischer titrations as well as for potential measurements.



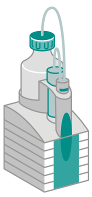
901 Titrando

The titrator can be used for volumetric Karl Fischer titrations, endpoint titrations as well as pH value, potential and temperature measurements.



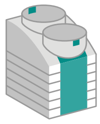
902 Titrando

The titrator can be used for endpoint titrations, pH value, potential and temperature measurements as well as enzymatic and STAT titrations.



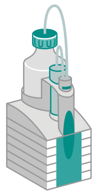
904 Titrando

The titrator can be used for potentiometric and voltametric titrations, endpoint titrations as well as concentration, pH value, potential and temperature measurements.



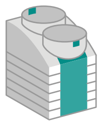
905 Titrando

The titrator can be used for potentiometric and voltametric titrations, endpoint titrations as well as concentration, pH value, potential and temperature measurements.



906 Titrando

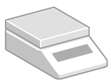
The titrator can be used for potentiometric and voltametric titrations, endpoint titrations, volumetric Karl Fischer titrations as well as concentration, pH value, potential and temperature measurements.



907 Titrando

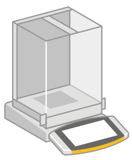
The titrator can be used for potentiometric and voltametric titrations, endpoint titrations, volumetric Karl Fischer titrations as well as concentration, pH value, potential and temperature measurements.

Other instruments



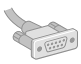
Balance

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

Functional unit – Directory (chapter 5.10.2.1, page 697)

Instruments – Status (chapter 5.10.1.2, page 665)

Instruments – Manual control (chapter 5.10.1.6, page 669)

Instruments – Properties (chapter 5.10.1.5, page 668)

Reserving instruments (chapter 5.10.1.3, page 666)

Releasing instruments (chapter 5.10.1.4, page 667)

Backing up instrument data (chapter 5.10.1.7, page 670)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

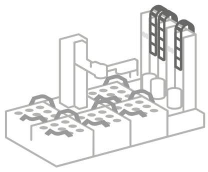
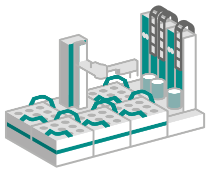
OMNIS Software – Inventory (chapter 5.2.2, page 99)

5.10.1.2 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 light. The color and the condition of the status light varies, depending on the status of the instrument.

The status of the instruments in the OMNIS Software is represented as follows:

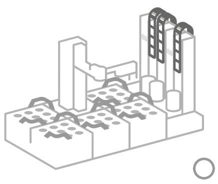
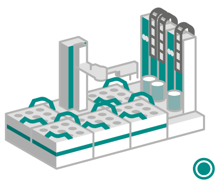
Display in the Inventory

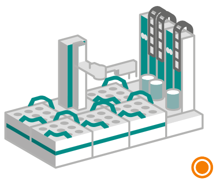
	The instrument is reserved by another OMNIS system and is thus not available.
	The instrument is available.

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.

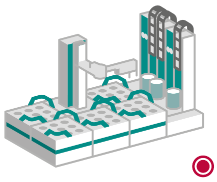
Other instruments such as balances or barcode readers can be assigned to several OMNIS systems at the same time.

	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 logging in is therefore possible.



The instrument is currently in the error state.

See also

Instruments – Directory (chapter 5.10.1.1, page 660)

Reserving instruments (chapter 5.10.1.3, page 666)

5.10.1.3 Reserving instruments

The instruments reserved for the user, together with their functional units and the additionally connected equipment (stirrers, solutions, sensors, sample racks, etc.) are displayed in the **Equipment** work area under **Instruments**.

1 Opening the instrument management

- Click on to open the **Inventory** window in **Equipment ▶ Instruments**.

The instruments available are displayed. The status of the instruments is represented thereby as follows: *Instruments – Status (see chapter 5.10.1.2, page 665)*

2 Instrument Search

- If necessary, click on if new instruments have been connected.
- Enter the desired search criterion (name, type, IP address) in the search field.

The instrument list will display only the instruments which contain the search term used.

3 Reserving instruments

- Insert the desired instruments from the instrument list per drag and drop into the area on the right.

NOTICE

- The instruments are reserved by the **Metrohm MIAMI LabLogic (Laboratory Logic service)**. This Windows system service is installed together with the OMNIS Software and starts automatically when starting Windows. This means that the instruments remain reserved when the OMNIS Software is exited. The instruments are released again as soon as Windows is exited or the **Metrohm MIAMI LabLogic service** is stopped.
- If the computer is switched on again and the OMNIS Software is started, the reserved instruments will be connected and initialized once again.
- If the running **Metrohm MIAMI LabLogic service** is stopped unexpectedly, e.g. due to a power failure, instruments can sometimes not be found anymore in the network. In this case, this service needs to be restarted under "Services" in the Windows Task Manager. Then a search for instruments on the network can be started again and they can be reserved.

See also

Releasing instruments (chapter 5.10.1.4, page 667)

5.10.1.4 Releasing instruments

The instruments reserved for the user can be released again in the **Equipment** work area under **Instruments** and made available for other users.

Proceed as follows to release reserved instruments:

1 Opening the instrument management

- In the **Equipment** work area, click on the **Instruments** subsection.

2 Releasing the instrument

- Click on the desired instrument.
- Remove the selected instrument by clicking on ✕.

The instrument is released and is once again available for other users.

See also

Reserving instruments (chapter 5.10.1.3, page 666)

5.10.1.5 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	Type of product (English designation).

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 internal IT administrator.

Specific data

Specific settings can also be made in this subsection if a functional unit has been selected.

NOTICE

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.

NOTICE

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.

See also

Backing up instrument data (chapter 5.10.1.7, page 670)

Collecting instrument log files (chapter 10, page 956)

5.10.1.6 Instruments – Manual control

Manual control makes it possible to actuate a reserved instrument directly, i.e. without predefined operating procedure. The prerequisites for this are:

- The instrument is switched on.
- The instrument is recognized by the software.
- 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

To initialize the instrument, click the following icon:

	Initialize the instrument.

See also

Sample robot – Manual control (chapter 5.10.1.9, page 672)

Functional unit – Manual control (chapter 5.10.2.5, page 708)

5.10.1.7 Backing up instrument data

> **NOTICE**
>
> 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.

NOTICE

The directory with the backup files is hidden by default in Windows.

Restoring the instrument data must be carried out by the internal IT administrator.

NOTICE

Repeat the steps 1 to 4 for all available instruments.

See also

Instruments – Definition (chapter 5.10.1, page 660)

Instruments – Properties (chapter 5.10.1.5, page 668)

5.10.1.8 Sample robot – Properties / Specific data

If an instrument of the **OMNIS Sample Robot** type is selected in the instrument overview, the specific product information and settings for the instrument appear in the **Specific data** subsection of the **Properties** window.

Product information	
Product name	Name of the OMNIS Sample Robot. This name is saved onto the integrated chip of the sample robot.
Product type	Type of the product (English designation).

Production data	
Article number	Number that identifies the product unambiguously.
Serial number	Serial number of the product.

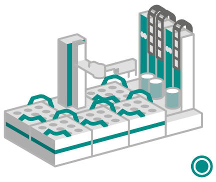
See also

Sample robot – Manual control (chapter 5.10.1.9, page 672)

5.10.1.9 Sample robot – Manual control

If an instrument of the **OMNIS Sample Robot** type is selected in the **Instruments** subsection, this instrument can be initialized in the **Manual control** window.

Status display



The current status of the sample robot is visible in the icon display.

Initializing

	Click this icon to initialize the sample robot with all associated functional units. During the initialization, the status symbol of the sample robot flashes **orange**. As soon as all of the associated functional units have been initialized, the status symbol will light up **green**.

NOTICE

The entire gripper arm of the sample robot must be within the instrument limit for the instrument to be initialized. The instrument limits are defined by the rack base.

If the gripper arm is outside this range, then it needs to be manually moved back into this range.

See also

Main module Pick&Place – Manual control (chapter 5.10.2.16, page 745)

Pick&Place module – Manual control (chapter 5.10.2.22, page 752)

Pump module – Manual control (chapter 5.10.2.38, page 765)

5.10.1.10 874 Oven Sample Processor – Faults

If an unknown 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 applying the measures suggested in the error message, contact must be made with the regional Metrohm representative. The following instrument malfunctions may occur:

Error code	Cause
013-001-1-255	Communication problems exist between the oven module and the sample changer.
013-002-1-255	The data of the oven module 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 module – Properties (chapter 5.10.2.18, page 748)

5.10.1.11 Serial instrument – Properties / Specific data

If an instrument of the **Serial device** type is selected in the instrument overview, the specific settings for the instrument appear in the **Specific data** subsection of the **Properties** window.

RS-232 configuration	
COM port	Display the serial interface on the PC 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 itself.
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

Instruments – Properties (chapter 5.10.1.5, page 668)

Configuring the balance (chapter 5.10.1.15, page 680)

5.10.1.12 Spektrometer – Properties

Clicking on under **Equipment ▶ Instruments** opens the **Properties** window.

General

The product information and production data of the measuring unit of the spectrometer are displayed in the **General** subsection: *Instruments – Properties (see chapter 5.10.1.5, page 668)*.

Specific data

The following functions and information are available for instruments of the **2060 the NIR** type in the subsection **Specific data**:

Channel 1 … 5	
Measuring mode	Select measuring mode or deactivate 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: ▪ 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 glass fiber unambiguously.
Fiber length	Enter the length of the fiber optic cable used.

NOTICE

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.

See also

MEAS SPEC – Properties (chapter 5.9.4.12.7, page 502)

Command – Directory (chapter 5.9.4.17, page 622)

5.10.1.13 Cubis II balance – Properties / Specific data

If an instrument of the **Cubis II balance** type is selected in the instrument overview, the specific settings for this balance appear in **Properties ▶ Specific data**.

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 5.10.1.5, page 668)

Operating the Cubis II balance (chapter 5.10.1.16, page 682)

5.10.1.14 Balance – Properties / Specific data

If an instrument of the **Balance** type is selected in the instrument overview, the specific settings for the balance appear in **Properties ▶ Specific data**.

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.

<table>
<tr><th colspan="2">User-defined</th></tr>
<tr><td>Weighing response pattern</td><td>Pattern which is looked for in the response of the balance to the weighing command that was sent. At least 2 groups must be defined: One for the weight (?<value>) and one for the unit (?<unit>). Optionally, a group for the algebraic sign (?<sign>) can be defined. After the group definition, the corresponding RegEx expression must be entered:
▪ Weight as numerical value with decimal place: (?<value>\d+\.\d+)
▪ Unit, e.g. for grams: (?<unit>[g])
▪ Optionally, algebraic sign 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.

RegEx – Regular expression (see chapter 5.9.5.5.19, page 655)</td></tr>
<tr><td>Tare</td><td>The signs defined here are sent to the balance with the TARE command. Consult the instructions for the balance.</td></tr>
<tr><td>Tare response pattern</td><td>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.

RegEx – Regular expression (see chapter 5.9.5.5.19, page 655)</td></tr>
</table>

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 5.10.1.15, page 680)

Instruments – Properties (chapter 5.10.1.5, page 668)

5.10.1.15 Configuring the balance

NOTICE

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: *Operating the Cubis II balance (see chapter 5.10.1.16, page 682)*

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: *Instruments – Properties (see chapter 5.10.1.5, page 668)*
  - 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: *Cubis II balance – Properties / Specific data (see chapter 5.10.1.13, page 676)*
  Cubis II balance – Properties / Specific data (see chapter 5.10.1.13, page 676)

  Balance – Properties / Specific data (see chapter 5.10.1.14, page 676)
  - 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.

> **NOTICE**
>
> 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

Instruments – Properties (chapter 5.10.1.5, page 668)

Cubis II balance – Properties / Specific data (chapter 5.10.1.13, page 676)
Cubis II balance – Properties / Specific data (chapter 5.10.1.13, page 676)

Balance – Properties / Specific data (chapter 5.10.1.14, page 676)

Operating the Cubis II balance (chapter 5.10.1.16, page 682)

WEIGH – Parameters (chapter 5.9.4.16.21, page 620)

WEIGH – Command variables (chapter 5.9.4.16.22, page 621)

5.10.1.16 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. Observe in this connection the corresponding instructions in the **Technical White Paper** in the *Metrohm Knowledge Base*.

> **NOTICE**
>
> 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 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 **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 PC name of the desired OMNIS-system.

The login window is displayed.

2 User login

- Enter login information for the OMNIS system.

The balance is connected with the OMNIS system and the available work sequences are displayed.

NOTICE

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.
- **Weighing-in via REQUEST**: 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).

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.

NOTICE

The search function can be filtered directly for suitable sample lists.

3 Selecting a sample

- Select the desired sample in the display.

NOTICE

The search function can be filtered directly for suitable samples. A barcode reader can be used as the input device 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.
- Sample rack on which the sample is located if this has been defined in the OMNIS Software.
- Sample position of the sample in the sample 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.

NOTICE

The search function can be filtered directly for suitable subsamples. A barcode reader can be used as the input device 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.
- Sample rack on which the subsample is located if this has been defined in the OMNIS Software.
- Sample position of the subsample in the sample 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. At the time of the weighing, a graphic signal indicates whether the measured value falls within the valid range between the minimum and maximum values. 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 dispatch the weight to the OMNIS Software via the orange **+** button.

If the 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 in the input fields of the selected subsample, this will be signaled by an error message.

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.

Weigh in by REQUEST

Prerequisite:

- The execution of the subsample with a **REQUEST** command must be ongoing and the **REQUEST** 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.

NOTICE

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.

NOTICE

If multiple **REQUEST** commands are processed in a method, then the subsample must be updated after the recording of the weight so that the next command will be available for selection.

2 Select REQUEST

- 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 dispatch the weight to the OMNIS Software via the orange **+** button.

If the receipt of the weighing by difference data is successful, then this will be signaled 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 in the input fields of the selected subsample, this will be signaled by an error message.

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

1 Selecting work sequences

- On the display, select the **Control with OMNIS Software** work sequence.

The balance is now available only for commands of the **WEIGH** and **TARE** type which are being run in an ongoing operating procedure on the connected OMNIS system.

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.

Carrying over weighing data to subsamples (see chapter 5.8.5.3, page 186)

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, including a reason for why it failed if appropriate.
- 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
  - Hostname 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 logoff or every interruption of the connection between the OMNIS Software and the balance is recorded in an entry.

- The following information is recorded when a subsample is weighed in or weighed by difference
  - Balance (hostname) from which the weighing 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.

NOTICE

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 subsection **History**:

- 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

Instruments – Properties (chapter 5.10.1.5, page 668)

Cubis II balance – Properties / Specific data (chapter 5.10.1.13, page 676)
Cubis II balance – Properties / Specific data (chapter 5.10.1.13, page 676)

Balance – Properties / Specific data (chapter 5.10.1.14, page 676)

5.10.1.17 Metrohm USB devices – Troubleshooting

Known bugs and restrictions

NOTICE

When connecting Metrohm USB devices to an OMNIS system in a centrally managed network, we recommend to **deactivate the sleep options** in Microsoft Windows with group policy for the computer used and the USB connector.

When using Metrohm USB device in the OMNIS Software, the following errors can occur:

- *Connection errors when connecting several Metrohm USB devices*
- *The instrument is not displayed correctly in the Inventory after exiting the sleep mode of the computer and removing a Metrohm USB device*
- *The device is not displayed correctly in the Inventory after exiting the sleep mode or the hibernate mode of the computer and adding a Metrohm USB device*
- *Incorrect display in the Inventory after OMNIS Software update with Metrohm USB device connected*
- *Errors in Windows 10 when using the fast startup function*
- *Errors with USB device driver, COM ports and USB devices are not found*

Connection errors when connecting several Metrohm USB devices

A Metrohm USB device is connected and assigned to the computer on which the OMNIS Software is installed.

1. Several Metrohm USB devices are connected with one another via the USB connector of the Metrohm USB device.
2. The instrument is removed from the computer and connected again.
3. The **Equipment ▶ Instruments ▶ Inventory** window opens.
4. The assignment of the Metrohm USB devices is removed.

An error occurs when trying to reassign the Metrohm USB device.

Troubleshooting

1 Click on to open the **Inventory** window in **Equipment ▶ Instruments**.

The Metrohm USB device can now be used again by the OMNIS Software.

The instrument is not displayed correctly in the Inventory after exiting the sleep mode of the computer and removing a Metrohm USB device

A Metrohm USB device is connected and assigned to the computer on which the OMNIS Software is installed.

1. The computer enters the sleep mode.
2. The computer is restarted from the sleep mode.
3. The assignment of the Metrohm USB device is removed.
4. The Metrohm USB device is disconnected from the USB connector of the computer.

Although the Metrohm USB device is not connected to the USB connector of the computer, it is displayed in the **Equipment ▶ Instruments ▶ Inventory** window.

NOTICE

The error occurs because the **Metrohm OMNIS DeviceServer** service is in a faulty status. As a consequence, devices are not grayed out after being removed from the network or the computer. The Metrohm USB devices are still displayed as available in the **Inventory** even though they are neither connected nor assigned.

Troubleshooting

1 Restart the computer.

2 Click on the icon to open the **Inventory** window in **Equipment ▶ Instruments**.

The Metrohm USB device is no longer displayed in the **Inventory**.

The device is not displayed correctly in the Inventory after exiting the sleep mode or the hibernate mode of the computer and adding a Metrohm USB device

A Metrohm USB device is connected and assigned to the computer on which the OMNIS Software is installed.

1. The computer enters the sleep mode or the hibernate mode.
2. The computer is restarted from the sleep mode or the hibernate mode.
3. Another Metrohm USB device is connected.

The Metrohm USB device is not displayed in the **Equipment ▶ Instruments ▶ Inventory** window, even though it is connected.

NOTICE

The error occurs because the **Metrohm OMNIS DeviceServer** service is in a faulty status. As a consequence, newly connected Metrohm USB devices are not displayed in the **Inventory**.

Troubleshooting

1. Restart the computer.
2. Click on ☰ to open the **Inventory** window in **Equipment ▶ Instruments**.

   The connected Metrohm USB device is displayed correctly in the **Inventory**.

Incorrect display in the Inventory after OMNIS Software update with Metrohm USB device connected

A Metrohm USB device is connected to the computer on which the OMNIS Software is installed.

1. An OMNIS Software update is installed on the computer.
2. A restart is required and the computer is restarted.

The Metrohm USB device is not displayed in the **Equipment ▶ Instruments ▶ Inventory** window, even though it is connected.

NOTICE

The error occurs because the **Metrohm OMNIS DeviceServer** service is in a faulty status. As a consequence, newly connected Metrohm USB devices are not displayed in the **Inventory**.

Troubleshooting

1. Reinstall the OMNIS Software in repair mode.
2. Click on ☰ to open the **Inventory** window in **Equipment ▶ Instruments**.

The connected Metrohm USB device is displayed correctly in the **Inventory**.

Errors in Windows 10 when using the fast startup function

A Metrohm USB device is connected and assigned to the computer on which the OMNIS Software is installed.

1. The computer is shut down.
2. The computer is started up.
3. The Metrohm USB device is disconnected from the USB connector of the computer.

The Metrohm USB device is still displayed as connected in the **Equipment ▶ Instruments ▶ Inventory** window even though it is not connected.

NOTICE

The error occurs because the **Metrohm OMNIS DeviceServer** service is in a faulty status. As a consequence, devices are not grayed out after being removed from the network or the computer. The Metrohm USB devices are still displayed as available in the **Inventory** even though they are neither connected nor assigned.

Troubleshooting

1 Restart the computer.

2 Connect the same Metrohm USB device to the computer again.

3 Click on to open the **Inventory** window in **Equipment ▶ Instruments**.

4 Remove and restore the assignment of the Metrohm USB device.

Click on to update the Inventory.

The connected Metrohm USB device is displayed correctly in the **Inventory**.

Errors with USB device driver, COM ports and Metrohm USB devices are not found

A Metrohm USB device is connected and assigned to the computer on which the OMNIS Software is installed.

1. A search is carried out in **Equipment ▶ Instruments ▶ Inventory** for COM ports or Metrohm USB devices, but none is found.

NOTICE

The error occurs because the **Metrohm OMNIS DeviceServer** service is in a faulty status. As a result, COM ports and Metrohm USB devices are not found in the **Inventory**.

No Metrohm USB devices are found in the OMNIS Software at the time of installation of the OMNIS Software with the USB device driver from Thesycon, with version 3.12 and subsequent installation, e.g. of MagIC Net with the USB device driver with version 2.51.

Furthermore, this problem also occurs with the following versions and earlier: viva 2.0, MagIC Net 3.2, Tiamo 2.5, StabNet 1.1, TiBase 1.1 and 797 VA Computrace 1.3.

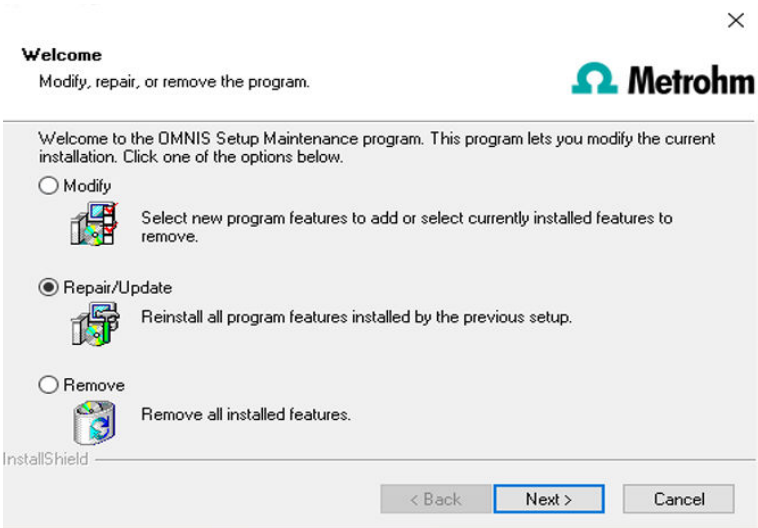
Troubleshooting

1 In the program directory **C:\Program Files\Metrohm\metr_770**, uninstall the USB device driver **uninstall.exe**.

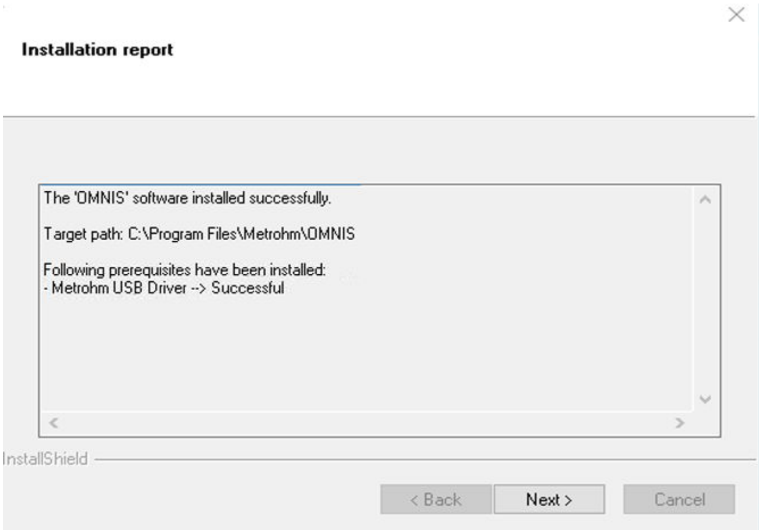
2 Restart the computer.

3 Install the OMNIS Software once again, while at the same time starting the **OMNIS-Desktop-Setup_....exe** program on the storage medium.

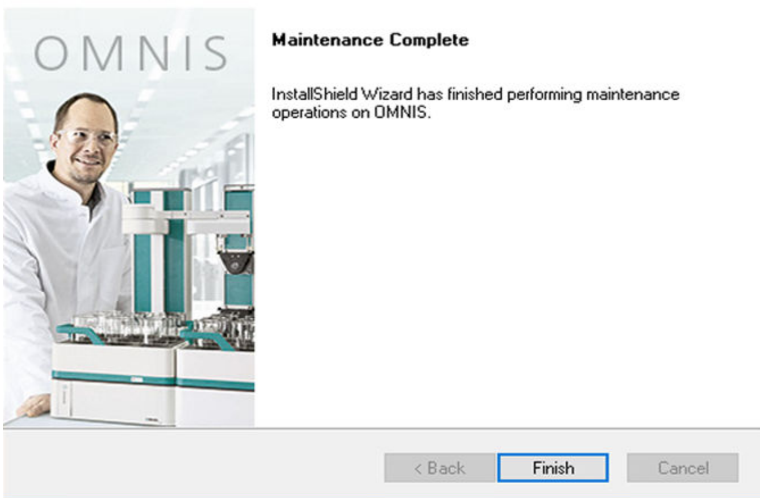
4 Select the **[Repair/Update]** function and confirm with **[Next>]**.



5 An installation report is created at the end of the installation process. Check the content of the report and confirm with **[Next>]**.



6 Complete the installation with **[Finish]**.



7 Open the OMNIS Software. Click on to open the **Inventory** window in **Equipment ▶ Instruments**.

8 Click on to update the Inventory.

The Metrohm USB devices are displayed in the **Inventory**.

See also

805 Dosimat – Properties / Specific data (chapter 5.10.2.6, page 710)

805 Dosimat – Properties / Specific data (chapter 5.10.2.6, page 710)

Dosing device (MSB) – Properties / Specific data (chapter 5.10.2.7, page 711)

Dosing unit (OMNIS) – Properties / Specific data (chapter 5.10.2.8, page 715)

Instruments – Properties (chapter 5.10.1.5, page 668)

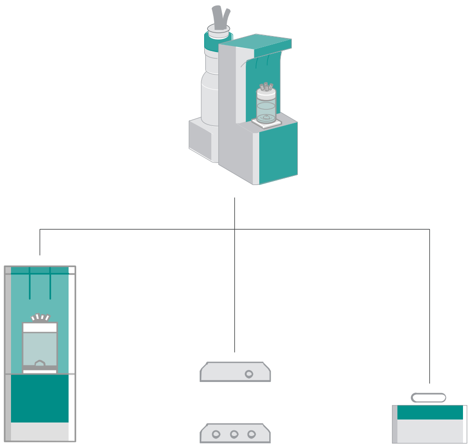
Measuring interface – Properties (chapter 5.10.2.17, page 747)

5.10.2 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

Functional unit – Directory (chapter 5.10.2.1, page 697)

Functional unit – Status (chapter 5.10.2.2, page 705)

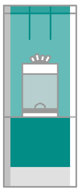
Functional unit – Manual control (chapter 5.10.2.5, page 708)

Assigning functional units to a command (chapter 5.10.2.3, page 706)

5.10.2.1 Functional unit – Directory

- *Functional units of OMNIS instruments*
- *Functional units of Metrohm USB instruments*
- *Functional units of other instruments*

Functional units of OMNIS instruments



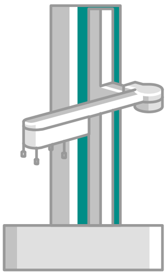
Dosing drive

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.

Magnetic Stirrer

The functional unit can be part of the following instruments and modules: **OMNIS Titrator**, **OMNIS Titration Module**, **OMNIS Dosing 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.

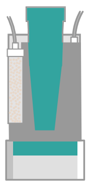
The following sensor types are available: Temperature sensor, pH electrode, metal electrode, polarizable metal electrode, ion-selective electrode and other sensor.

Measuring Module 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 and ion-selective electrode.

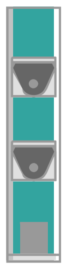
OMNIS Rod Stirrer

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.



Peristaltic pump

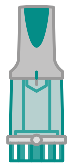
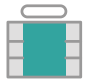
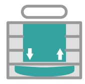
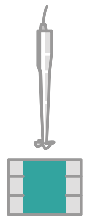
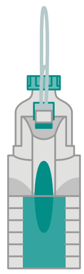
The functional unit is installed in the **Pump Module** of a sample robot and can be used for various liquid handling tasks (e.g. aspiration or rinsing). A pump module is equipped with either 2 or 4 peristaltic pumps.

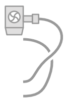
Pick&Place module

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.

Functional units of Metrohm USB devices

	**800 Dosino** The functional unit can be connected to the MSB connectors of Metrohm USB devices. 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 devices.
	**803 Ti Stand** The functional unit is connected to the MSB connectors of Metrohm USB devices. 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 devices. 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 devices. 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.



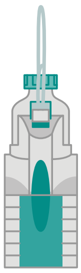
Gas flow module

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 module**. 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

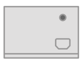
The functional unit is installed in instruments of the **902 Titrando** type. The functional unit is used as a measuring interface for analog sensors.

The following sensor types are available: Temperature sensor, pH electrode, metal electrode, ion-selective electrode and other electrode.

Measuring interface analog

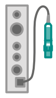
The functional unit is installed in instruments of the **888 Titrando**, **901 Titrando**, **904 Titrando**, **905 Titrando**, **906 Titrando** and **907 Titrando** type. The functional unit is used as a measuring interface for analog sensors.

The following sensor types are available: temperature sensor, pH electrode, metal electrode, polarizable metal electrode, ion-selective electrode and other electrode.



Measuring interface conductivity

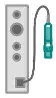
The functional unit is installed in instruments of the **856 Conductivity Module** type. The functional unit is used as a measuring interface for analog sensors of the conductivity measuring cell type.



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 **888 Titrando**, **901 Titrando**, **904 Titrando**, **905 Titrando**, **906 Titrando** and **907 Titrando** type.

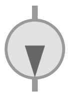
The **Measuring interface iConnect** is used as a measuring interface for sensors of the **iTrode** type. The following sensor types are available: pH electrode and metal electrode.



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.

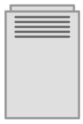


Membrane pump (aspirate)

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.

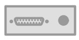
Membrane pump (rinse)

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.



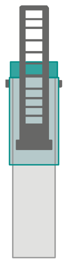
Oven module

The functional unit is installed in instruments of the **874 Oven Sample Processor** type and is part of the **Oven & gas flow module**. The functional unit is used for software-controlled temperature control for heating the sample vessel.



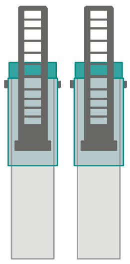
Remote Box MSB

The functional unit can be connected to the MSB connectors of Metrohm USB devices. 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.



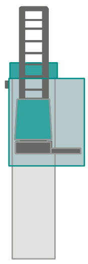
Tower

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.



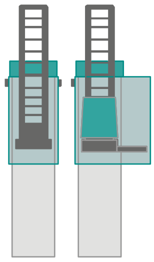
Tower

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.



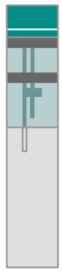
Tower + 786 Swing Head

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.



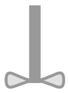
Tower + 786 Swing Head

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

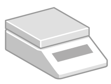
The functional unit is comprised of the tower and the turntable of the **874 Oven Sample Processor** and is used, together with the mounted **Sample processor rack**, for approaching sample vessels.



Tower stirrer socket

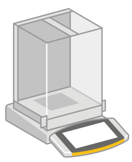
The functional unit is installed in the tower of instruments of the types **814 USB Sample Processor**, **815 Robotic USB Sample Processor XL** and **855 Robotic Titrosampler**. The functional unit is used as a connector and for the operation of an **802 Stirrer** or a **741 Magnetic Stirrer**.

Functional units of other instruments



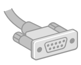
Balance

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

Functional unit – Status (chapter 5.10.2.2, page 705)

Functional unit – Manual control (chapter 5.10.2.5, page 708)

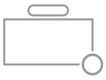
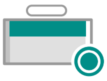
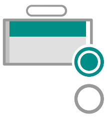
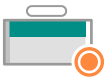
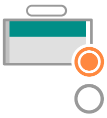
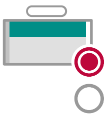
Assigning functional units to a command (chapter 5.10.2.3, page 706)

Additional component – Directory (chapter 5.10.4.1, page 789)

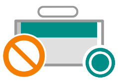
5.10.2.2 Functional unit – Status

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 initialized.
	(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.

NOTICE

Double-clicking on a connected functional unit opens the Manual control.

See also

Functional unit – Manual control (chapter 5.10.2.5, page 708)

Instruments – Status (chapter 5.10.1.2, page 665)

5.10.2.3 Assigning functional units 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 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 automatic assignment of the functional units is not possible, then they must be assigned to the commands manually. Please proceed as follows:

1 Opening command properties

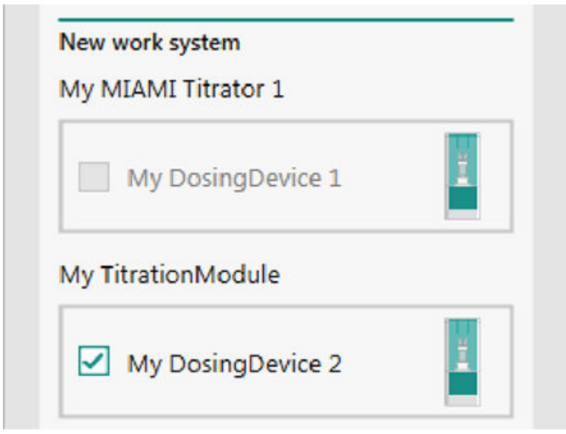
- Select the desired command in the method editor.
- Click on the icon to open the **Properties** window.
- Select the **Execute with** subsection.

2 Assigning functional unit manually

- Activate the check box next to the functional unit to assign it to the command.

NOTICE

The functional unit only needs to be assigned manually if more than one functional unit of the same type is contained in the work system. It will be assigned automatically when the functional unit is unambiguous.



NOTICE

The method cannot be started if a functional unit necessary for a command cannot be found in the work system. Therefore, ensure that the work system contains all the necessary functional units.

See also

Method – Definition (chapter 5.9.2, page 281)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

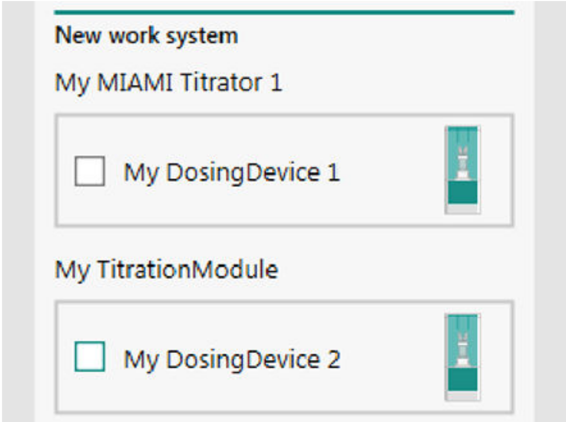
5.10.2.4 Removing assigned functional units from a command

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

Method – Definition (chapter 5.9.2, page 281)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

5.10.2.5 Functional unit – Manual control

Manual control makes it possible to actuate the functional units connected to the reserved instruments 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 software.
- The functional unit is not occupied by a process sequence.

NOTICE

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 manual control of the selected functional unit. As

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.
	Activate function.
	Deactivate function.
	Increase stirring rate.
	Reduce stirring rate.
	Activate **Park** function.

See also

805 Dosimat – Manual control (chapter 5.10.2.9, page 720)
805 Dosimat – Manual control (chapter 5.10.2.9, page 720)

800 Dosino – Manual control (chapter 5.10.2.10, page 722)

Dosing unit – Manual control (chapter 5.10.2.11, page 727)

801 Stirrer – Manual control (chapter 5.10.2.27, page 756)
801 Stirrer – Manual control (chapter 5.10.2.27, page 756)

Magnetic Stirrer – Manual control (chapter 5.10.2.28, page 757)

OMNIS Rod Stirrer – Manual control (chapter 5.10.2.24, page 754)

Main module Pick&Place – Manual control (chapter 5.10.2.16, page 745)

Pick&Place module – Manual control (chapter 5.10.2.22, page 752)

Pump module – Manual control (chapter 5.10.2.38, page 765)

5.10.2.6 805 Dosimat – Properties / Specific data

Clicking on under **Equipment ▶ Instruments** opens the **Properties** window. The following functions and information are available for the 2 components **806 Exchange Unit** and **805 Dosimat** (dosing drive) 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.

Connection	
MSB connector	Display the number of the MSB connector on the Metrohm USB device that the functional unit is connected to.

See also

Instruments – Directory (chapter 5.10.1.1, page 660)

805 Dosimat – Manual control (chapter 5.10.2.9, page 720)
805 Dosimat – Manual control (chapter 5.10.2.9, page 720)
800 Dosino – Manual control (chapter 5.10.2.10, page 722)

Dosing unit – Manual control (chapter 5.10.2.11, page 727)

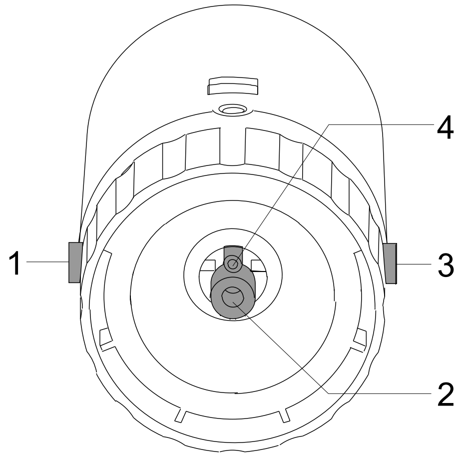
Instruments – Properties (chapter 5.10.1.5, page 668)

5.10.2.7 Dosing device (MSB) – Properties / Specific data

If a functional unit of the **800 Dosino** type is selected in the overview list, the specific data for the two components **807 Dosing Unit** and **800 Dosino** (dosing drive) appears in **Equipment ► Instruments ► Properties ► Specific data**.

807 Dosing Unit

The **807 Dosing Unit** is equipped with a distributor with 4 connectors that are defined as 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 that is connected to the fill port of the dosing unit (in cm). 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 the **Fill port**. For the **Maximum filling rate**, the following rule applies: **Maximum filling rate** = **10/3*cylinder volume**. In addition, the instrument checks that this rate does not exceed 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** has to 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 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 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 that this rate does not exceed 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** has to 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 is connected to dosing port 2 of the dosing unit (in cm). 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 that this rate does not exceed 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** has to 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 that is connected to the special port of the dosing unit (in cm). 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 that this rate does not exceed 10/3 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate.

NOTICE

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 software to calculate the required volume for the preparation and the emptying automatically. 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** The opening of the valve disk may not rotate via the port that is selected in the **Do not rotate over** field. In this way, contamination caused by dripping is avoided.
Do not rotate over	Selection of the port that is not to be traversed when the valve disk is rotated.

Cylinder	Information on the glass cylinder in the dosing unit.
Cylinder volume	Volume of the cylinder inserted in the dosing unit.

Cylinder	Information on the glass cylinder 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.

Connection	
MSB connector	Number of the MSB connector on the Metrohm USB device that the functional unit is connected to.

See also

Instruments – Directory (chapter 5.10.1.1, page 660)

805 Dosimat – Manual control (chapter 5.10.2.9, page 720)
805 Dosimat – Manual control (chapter 5.10.2.9, page 720)
800 Dosino – Manual control (chapter 5.10.2.10, page 722)

Dosing unit – Manual control (chapter 5.10.2.11, page 727)

Instruments – Properties (chapter 5.10.1.5, page 668)

5.10.2.8 Dosing unit (OMNIS) – Properties / Specific data

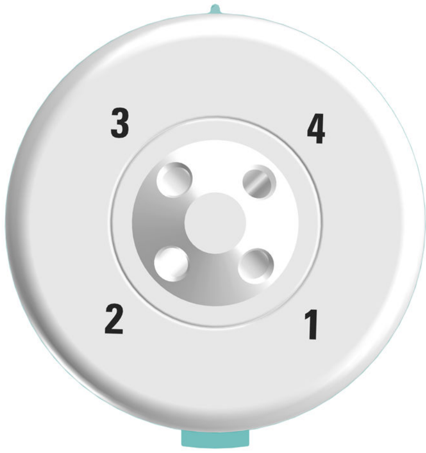
If a functional unit of the **Dosing unit** type is selected in the overview of the instrument, then the specific settings for the **Cylinder unit** in the dosing unit are displayed in the **Specific data** subsection of the **Properties** window.

NOTICE

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 connectors that are referred to as 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 use of the ports 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 verifies that this rate is not bigger 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 (mm).
Maximum dosing rate	Maximum permissible rate for dosing. In addition, the instrument verifies that this rate is not bigger 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** has to be reduced if highly viscous solutions are dosed or if tubing thinner than the standard tubing is used.

NOTICE

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 verifies that this rate is not bigger 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** has to 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 verifies that this rate is not bigger than 6 times the cylinder volume per minute. If this should be the case, then the instrument will reduce the rate.

NOTICE

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 software to calculate the required volume for the preparation and the emptying automatically. The preparation or the 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** The valve disk opening is not allowed to rotate via the port that is selected in the **Do not rotate over** field.
Do not rotate over	Selection of the port that is not to be traversed when the valve disk is rotated.

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

Instruments – Directory (chapter 5.10.1.1, page 660)

805 Dosimat – Manual control (chapter 5.10.2.9, page 720)

805 Dosimat – Manual control (chapter 5.10.2.9, page 720)

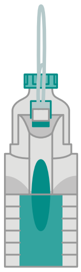
800 Dosino – Manual control (chapter 5.10.2.10, page 722)

Dosing unit – Manual control (chapter 5.10.2.11, page 727)

5.10.2.9 805 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.

NOTICE

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.

NOTICE

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.

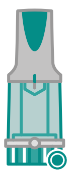
See also

Instruments – Properties (chapter 5.10.1.5, page 668)

5.10.2.10 800 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.

NOTICE

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.

NOTICE

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.

NOTICE

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 ASPI-RATE)	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

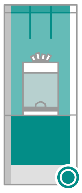
Instruments – Properties (chapter 5.10.1.5, page 668)

Operating the 800 Dosino (chapter 5.10.2.12, page 735)

5.10.2.11 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 …**)

Initializing

	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, fluid 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.

NOTICE

For a dosing unit that has not been initialized, only the functions **Initialize** and **Exchange position** are available in manual control. In the **Exchange position**, the cylinder unit can be removed (e.g. to remove jamming).

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.

NOTICE

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	Activate 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.

NOTICE

Fluid can escape when preparing the dosing unit. To avoid this, proceed as follows:

- Check if 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 dosing unit 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 dosing unit will be used.

	Click this icon to cancel the process.

NOTICE

To empty, remove the dosing unit from the bottle. Fluid can escape when emptying the dosing unit. To avoid this, proceed as follows:

- Check if all buret tips are pointing into a provided container.
- 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.

NOTICE

Before starting the **Exchange position** function, execute the **Empty** function. This ensures that fluids are no longer in the cylinder unit.

Function	Activate 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, the following specific parameters appear: – **Dosing port** – **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 (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 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 (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 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, the following specific parameters appear:
	  – **Aspiration volume**
	  – **Aspiration rate**
	  – **Aspiration port**
	  – **Dispensing rate**
	  – **Dispensing port**

Fill level (only for FILL)	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 (only for ASPIRATE)	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**	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 is to be moved.

Dispensing rate (only for ASPI-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 (only for ASPI-RATE)	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

Instruments – Properties (chapter 5.10.1.5, page 668)

805 Dosimat – Properties / Specific data (chapter 5.10.2.6, page 710)
805 Dosimat – Properties / Specific data (chapter 5.10.2.6, page 710)

Dosing device (MSB) – Properties / Specific data (chapter 5.10.2.7, page 711)

Dosing unit (OMNIS) – Properties / Specific data (chapter 5.10.2.8, page 715)

Functional unit – Status (chapter 5.10.2.2, page 705)

5.10.2.12 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**:

- *Operating the 800 Dosino (see chapter 5.10.2.12, page 735)*
  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 736)*
  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 737)*
  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 738)*
  The function is required if **807 Dosing Unit** is to be used with another solution.

NOTICE

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 the manual control icon 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.

NOTICE

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**.

NOTICE

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.

NOTICE

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 [icon] 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 [icon] 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 [icon] to start the **Empty** function.
- Observe the warning and click on **[Execute]** to confirm.

NOTICE

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 [icon] 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.

NOTICE

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

Reserving instruments (chapter 5.10.1.3, page 666)

Releasing instruments (chapter 5.10.1.4, page 667)

Instruments – Directory (chapter 5.10.1.1, page 660)

Functional unit – Status (chapter 5.10.2.2, page 705)

5.10.2.13 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 this tutorial, two variants are described to create a corresponding method:

- *Download a method as a template and use 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: *Creating and editing a method (see chapter 5.9.2.3, page 284)*

- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

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. *Importing the templates (see chapter 3.2, page 11)*

NOTICE

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. *Creating and editing an operating procedure (see chapter 5.9.1.3, page 265)*

NOTICE

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: *Creating and editing a method (see chapter 5.9.2.3, page 284)*

- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Creating a new method

- Create a new method or open an existing method in **Processes ▶ Methods**. *Creating and editing a method (see chapter 5.9.2.3, page 284)*
- 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**:
- Select the **Absolute** option in the **Target position** field.
- 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**). *Case – Condition (see chapter 5.9.5.5.17, page 654)*, *PISTON POS – Command variables (see chapter 5.9.4.14.13, page 560)*

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. *Creating and editing an operating procedure (see chapter 5.9.1.3, page 265)*

NOTICE

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. Further information on the **IF** command: *IF – Parameters (see chapter 5.9.4.16.5, page 595)*

See also

Creating and editing an operating procedure (chapter 5.9.1.3, page 265)

Creating a work system (chapter 5.10.3.2, page 785)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

Assigning functional units to a command (chapter 5.10.2.3, page 706)

5.10.2.14 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.

NOTICE

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 – Run (chapter 5.9.4.2.6, page 379)

STAT – Principle (chapter 5.9.4.2.4, page 369)

5.10.2.15 Main module Pick&Place – Properties / Specific data

If a functional unit of the **Main module Pick&Place** type is selected in the instrument overview, then the specific product information and production data for the main module Pick&Place appear in the **Specific data** subsection of the **Properties** window.

Product information	
Product name	Name of the main module. This name is written onto the memory chip of the sample robot.
Product type	Type of product (English designation).

Production data	
Article number	Number that identifies the product unambiguously.
Serial number	Serial number of the product.

NOTICE

Modified data of the functional unit cannot be saved for as long as it is being used by a method in the process sequence.

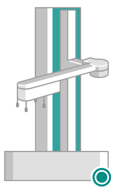
See also

Main module Pick&Place – Manual control (chapter 5.10.2.16, page 745)

5.10.2.16 Main module Pick&Place – Manual control

If a functional unit of the **Manual control** type is selected in the **Instruments** subsection, then the possible functions and parameters for the functional unit appear in the **Main module Pick&Place** window.

Status display



The current status of the main module is visible in the icon display.

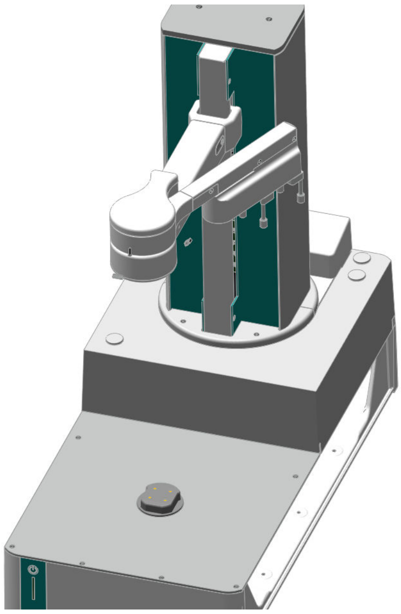
Initializing

Click this icon to initialize the Pick&Place main module.

During the initialization, the status symbol of the sample robot flashes **orange**. As soon as the main module Pick&Place is initialized, the status symbol lights up **green**.

If initialization is not possible, then the main module must be moved manually into initialization position.

Parking the robot arm



Click this icon to move the sample robot into park position. This ensures safe access to the work area during ongoing operation (e.g. to exchange racks).

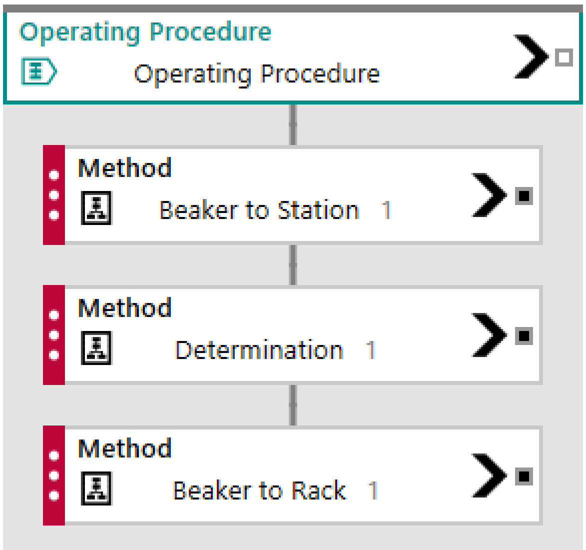
The robot arm moves into park position as soon as the operating procedure allows for it. A message indicates when the park position has been reached and the access is safe. Running methods are not interrupted. Operating procedures only pause when the robot arm becomes free. The parking procedure can be interrupted at any time.

Release the robot arm after completing the manipulation (e.g. after changing the rack) to allow waiting samples to continue to be processed.

NOTICE

Racks that are used in the determination run and that are marked with the icon must not be changed as one or more samples of this rack are being processed and they have to be moved back to the rack.

The park command waits until the end of a method using the robot arm before moving to park position. To keep the waiting time until parking as short as possible, it is useful to divide the operating procedure into methods for transporting the beaker and into a method for the determination:



To prevent the slide of the Pick&Place module from moving to the front when exchanging the rack, the **SLIDE** command should be contained in the transport method.

See also

Pick&Place module – Manual control (chapter 5.10.2.22, page 752)

Pump module – Manual control (chapter 5.10.2.38, page 765)

5.10.2.17 Measuring interface – Properties

Clicking on under **Equipment ▶ Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. 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.

> **NOTICE**
>
> **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 5.10.1.5, page 668)

5.10.2.18 Oven & gas flow module – Properties

Clicking on [icon] under **Equipment ▶ Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. The following functions and information are available in the subsection **Specific data** for functional units of the **Oven & gas flow module** type (part of an **Oven module**):

> **NOTICE**
>
> No data is displayed for the **gas flow module**.

Specific data

Oven data	
Temperature correction	Enter the correction value for the measured temperature. The temperature of the oven module 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.

NOTICE

The functional units **Oven module** and **Gas flow module** are called **Oven & gas flow module** by default.

In order to clearly distinguish between the functional units, we recommend to change the product names accordingly.

See also

Karl Fischer titration volumetric – Properties (chapter 5.9.4.2.9.3, page 404)

TEMP – Properties (chapter 5.9.4.15.16, page 585)

FLOW – Properties (chapter 5.9.4.15.15, page 584)

5.10.2.19 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 appear in the **Manual control** window.

Status display

The current status of the oven is visible in the icon display. Additionally, the current temperature is displayed in the status window.

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 has to be heated.

See also

Instruments – Properties (chapter 5.10.1.5, page 668)

Oven & gas flow module – Properties (chapter 5.10.2.18, page 748)

5.10.2.20 Gas flow module – Manual control

If a functional unit of the **Gas flow 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 gas flow module is visible in the icon display. Additionally, the current **Flow rate** is displayed in the status window.

Operating

	The gas flow module is switched off. Click the switch to turn on the gas flow.
	The gas flow module is switched on and runs until it is switched off again. 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

Instruments – Properties (chapter 5.10.1.5, page 668)

Oven & gas flow module – Properties (chapter 5.10.2.18, page 748)

Oven module – Manual control (chapter 5.10.2.19, page 749)

5.10.2.21 Pick&Place module – Properties / Specific data

If a functional unit of the **Pick&Place module** type is selected in the instrument overview, the specific product information and settings for the Pick&Place module appear in the **Specific data** subsection of the **Properties** window.

Product information	
Product name	Name of the Pick&Place module. This name is written onto the integrated memory chip of the Pick&Place module.
Product type	Type of the product (English designation).

Production data	
Article number	Number that identifies the product unambiguously.
Serial number	Serial number of the product.

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**

NOTICE

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.

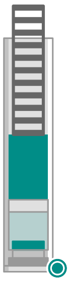
See also

Main module Pick&Place – Properties / Specific data (chapter 5.10.2.15, page 745)

5.10.2.22 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.

NOTICE

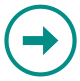
If the Pick&Place module has already been initialized, the icon is grayed out.

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 5.10.2.2, page 705)

5.10.2.23 OMNIS Rod Stirrer – Properties / Specific data

If a functional unit of the **OMNIS Rod Stirrer** type is selected in the overview of the instrument, then the specific product information and production data for the rod stirrer will appear in the **Specific data** subsection of the **Properties** window.

Operation of keys	Settings for the manual key operation 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.

NOTICE

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.

> **NOTICE**
>
> 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

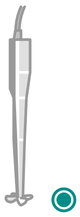
OMNIS Rod Stirrer – Manual control (chapter 5.10.2.24, page 754)

STIR – Properties (chapter 5.9.4.15.11, page 579)

5.10.2.24 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 5.10.2.2, page 705)

5.10.2.25 Magnetic Stirrer – Properties / Specific data

If a functional unit of the **Magnetic Stirrer** type is selected in the overview of the instrument, then the specific product information and production data for the magnetic stirrer will appear in the **Specific data** subsection of the **Properties** window.

Operation of keys	Settings for the manual key operation 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.

NOTICE

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 5.10.2.27, page 756)
801 Stirrer – Manual control (chapter 5.10.2.27, page 756)

Magnetic Stirrer – Manual control (chapter 5.10.2.28, page 757)

STIR – Properties (chapter 5.9.4.15.11, page 579)

5.10.2.26 801 Stirrer – Properties

Clicking on under **Equipment ▶ Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. The following functions and information are available for functional units of the **801 Stirrer** type in the **Specific data** subsection:

Specific data

Connection	
MSB connector	Number of the MSB connector on the Metrohm USB device that the functional unit is connected to.

See also

STIR – Properties (chapter 5.9.4.15.11, page 579)

5.10.2.27 801 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.

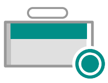
See also

801 Stirrer – Properties (chapter 5.10.2.26, page 756)

5.10.2.28 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.

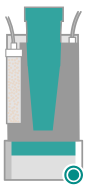
See also

Functional unit – Status (chapter 5.10.2.2, page 705)

5.10.2.29 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 5.10.1.5, page 668)

5.10.2.30 804 Ti Stand – Properties

Clicking on  under **Equipment ▶ Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. The following functions and information are available for functional units of the **804 Ti Stand** type in the **Specific data** subsection:

Specific data

Connection	
MSB connector	Number of the MSB connector on the Metrohm USB device that the functional unit is connected to.

See also

STIR – Properties (chapter 5.9.4.15.11, page 579)

5.10.2.31 803 Ti Stand – Properties

Clicking on  under **Equipment ▶ Instruments** opens the **Properties** window.

The product information and production data are displayed in the **General** subsection: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. The following functions and information are available for functional units of the **803 Ti Stand** type in the **Specific data** subsection:

Specific data

Connection	
MSB connector	Number of the MSB connector on the Metrohm USB device that the functional unit is connected to.

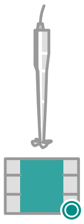
See also

STIR – Properties (chapter 5.9.4.15.11, page 579)

5.10.2.32 804 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.

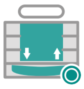
See also

Instruments – Properties (chapter 5.10.1.5, page 668)

5.10.2.33 803 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

804 Ti Stand – Properties (chapter 5.10.2.30, page 759)
804 Ti Stand – Properties (chapter 5.10.2.30, page 759)

803 Ti Stand – Properties (chapter 5.10.2.31, page 759)

5.10.2.34 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: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. 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 5.10.1.5, page 668)

PUMP – Properties (chapter 5.9.4.15.8, page 575)

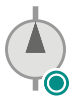
Membrane pump (rinse) – Manual control (chapter 5.10.2.35, page 762)
Membrane pump (rinse) – Manual control (chapter 5.10.2.35, page 762)

Membrane pump (aspirate) – Manual control (chapter 5.10.2.36, page 763)

5.10.2.35 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 5.10.2.2, page 705)

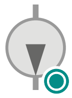
Instruments – Properties (chapter 5.10.1.5, page 668)

Membrane pump (aspirate) – Properties (chapter 5.10.2.34, page 762)

5.10.2.36 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 5.10.2.2, page 705)

Instruments – Properties (chapter 5.10.1.5, page 668)

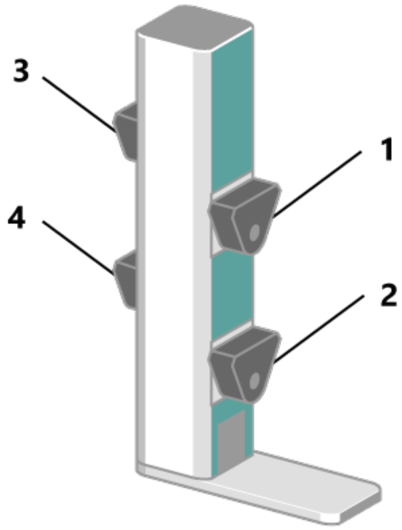
Membrane pump (aspirate) – Properties (chapter 5.10.2.34, page 762)

5.10.2.37 Pump module – Properties / Specific data

If a functional unit of the **Pump Module** type is selected in the instrument overview, the specific product information and settings for the pump module as well as the installed peristaltic pumps appear in the **Specific data** subsection of the **Properties** window.

The pump module is available in two different versions:

- **Pump module with 2 installed peristaltic pumps**
  The peristaltic pumps **1** and **2** are mounted on the front of the module.
- **Pump module with 4 installed peristaltic pumps**
  The peristaltic pumps **1** and **2** are mounted on the front of the module, peristaltic pumps **3** and **4** at the rear of the module.



The numbers of the peristaltic pumps can also be found on the pump module.

Pump Module

Information on the pump module is displayed in the **Specific data** subsection.

Product information	
Product name	Name of the pump module. This name is written onto the memory chip of the pump module.
Product type	Type of the product (English designation).

Production data	
Article number	Number that identifies the product unambiguously.
Serial number	Serial number of the product.

Peristaltic Pump 1 ... 4

Information on the individual peristaltic pumps is displayed in the **Specific data** subsection.

Product information	
Product name	Name of the peristaltic pump. This name is written onto the memory chip of the peristaltic pump.
Product type	Type of the product (English designation).

See also

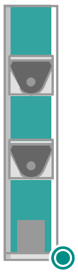
Pump module – Manual control (chapter 5.10.2.38, page 765)

PUMP – Properties (chapter 5.9.4.15.8, page 575)

5.10.2.38 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 5.10.2.2, page 705)

5.10.2.39 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: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. 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

Connection	
MSB connector	Number of the MSB connector on the MSB device that the functional unit is connected to.

See also

REMOTE IN – Properties (chapter 5.9.4.16.9, page 604)

REMOTE OUT – Properties (chapter 5.9.4.16.10, page 606)

5.10.2.40 Tower – Properties

Clicking on under **Equipment ▶ Instruments** opens the **Properties** window.

The product information is displayed in the **General** subsection: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. 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 highest position (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 activated, 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 deactivated, the sample rack is rotated to the starting position and the lift is moved to the home 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 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**.

Initial position	
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: 110 mm

See also

Defining the lift height (chapter 5.10.2.43, page 774)

Membrane pump (aspirate) – Properties (chapter 5.10.2.34, page 762)

External pump socket – Properties (chapter 5.10.2.45, page 780)

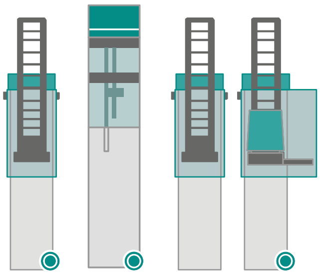
Tower stirrer socket – Properties (chapter 5.10.2.47, page 782)

Tower – Manual control (chapter 5.10.2.41, page 769)

5.10.2.41 Tower – Manual control

If a functional unit of the **Tower** type is selected in the **Instruments** sub-section, 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***Defining a special position (see chapter 5.10.2.44, page 778)*.
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: *Defining the lift height (see chapter 5.10.2.43, page 774)*.
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 5.10.2.2, page 705)

Tower – Properties (chapter 5.10.2.40, page 766)

5.10.2.42 786 Swing Head – Properties

Clicking on under **Equipment ▶ Instruments** opens the **Properties** window. The product information and production data are displayed in the **General** subsection: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. 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.

Robotic arm configuration	
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.
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.

NOTICE

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.

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 *Defining the lift height (see chapter 5.10.2.43, page 774)*.

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 *Defining the lift height (see chapter 5.10.2.43, page 774)*.

NOTICE

External positions are positions next to the sample rack, e.g. an external rinsing station.

See also

Functional unit – Directory (chapter 5.10.2.1, page 697)

Defining the lift height (chapter 5.10.2.43, page 774)

Tower – Manual control (chapter 5.10.2.41, page 769)

5.10.2.43 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.

> **NOTICE**
>
> 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.

> **NOTICE**
>
> 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

LIFT – Properties (chapter 5.9.4.15.4, page 566)

Sample rack – Properties (chapter 5.10.7.1, page 831)

Defining a special position (chapter 5.10.2.44, page 778)

Tower – Manual control (chapter 5.10.2.41, page 769)

5.10.2.44 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 .

NOTICE

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.

NOTICE

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.

NOTICE

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.

NOTICE

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 *Defining the lift height (see chapter 5.10.2.43, page 774)*.

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.

NOTICE

Up to 16 special positions can be defined for each sample rack.

See also

Defining the lift height (chapter 5.10.2.43, page 774)

MOVE TO RACK – Properties (chapter 5.9.4.15.6, page 571)

Sample rack – Properties (chapter 5.10.7.1, page 831)

5.10.2.45 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: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. 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.

> **NOTICE**
>
> 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

Functional unit – Directory (chapter 5.10.2.1, page 697)

Instruments – Properties (chapter 5.10.1.5, page 668)

PUMP – Properties (chapter 5.9.4.15.8, page 575)

External pump socket – Manual control (chapter 5.10.2.46, page 781)

5.10.2.46 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

Functional unit – Status (chapter 5.10.2.2, page 705)

Functional unit – Directory (chapter 5.10.2.1, page 697)

Instruments – Properties (chapter 5.10.1.5, page 668)

External pump socket – Properties (chapter 5.10.2.45, page 780)

5.10.2.47 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: *Instruments – Properties (see chapter 5.10.1.5, page 668)*. 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.

NOTICE

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.

NOTICE

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 5.10.1.5, page 668)

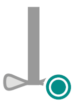
Tower stirrer socket – Manual control (chapter 5.10.2.48, page 782)

STIR – Properties (chapter 5.9.4.15.11, page 579)

5.10.2.48 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 5.10.2.2, page 705)

Instruments – Properties (chapter 5.10.1.5, page 668)

Tower stirrer socket – Properties (chapter 5.10.2.47, page 782)

5.10.3 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

OMNIS Software – Inventory (chapter 5.2.2, page 99)

Work system – Properties (chapter 5.10.3.1, page 784)

Creating a work system (chapter 5.10.3.2, page 785)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

Removing a work system from a method (chapter 5.10.3.4, page 787)

Functional unit – Manual control (chapter 5.10.2.5, page 708)

5.10.3.1 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.

NOTICE

- 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 5.10.3.2, page 785)

Work system – Definition (chapter 5.10.3, page 783)

5.10.3.2 Creating a work system

To create a new work system with functional units, instruments must already be reserved beforehand.

1 Setting up work system

- Click on in **Equipment ▶ Work systems**.

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 instruments 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 version of the method 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 the work system

- Save the work system by clicking on .

NOTICE

One functional unit can be assigned to several work systems.

NOTICE

If the selected work system is being used for conditioning, the current measured values for the ongoing conditioning process are displayed in **Current status**.

Further information on the conditioning: *Karl Fischer titration – Principle (see chapter 5.9.4.2.9.1, page 397)*
Karl Fischer titration – Principle (see chapter 5.9.4.2.9.1, page 397)

Conditioning – Principle (see chapter 5.9.4.2.9.2, page 402)

See also

Reserving instruments (chapter 5.10.1.3, page 666)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

Removing a work system from a method (chapter 5.10.3.4, page 787)

5.10.3.3 Assigning a work system to a method

By assigning work systems to methods, you define which functional units to use to run the individual commands within methods.

You can also assign multiple work systems to a method. This allows you to run commands of the same method with functional units of different work systems depending on the availability. This is particularly useful if you wish to perform the same analyses at several work stations of the sample robot.

To assign a work system to a method, proceed as follows:

1 Opening a method

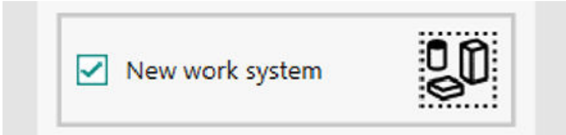
- In the **Processes** work area under **Methods**, select the desired method and open it with a double-click.

A new tab opens with the selected method as its title.

2 Assigning a work system

- Click to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

- Activate 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.

NOTICE

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

Creating a work system (chapter 5.10.3.2, page 785)

Removing a work system from a method (chapter 5.10.3.4, page 787)

Assigning functional units to a command (chapter 5.10.2.3, page 706)

Method – Properties (chapter 5.9.2.2, page 283)

Creating and editing a method (chapter 5.9.2.3, page 284)

5.10.3.4 Removing a work system from a method

To remove a work system from a method, proceed as follows:

1 Opening a method

- In the **Processes** work area under **Methods**, select the desired method and open it with a double-click.

A new tab opens with the selected method as its title.

2 Removing a work system

- Select the method by clicking the method icon.
- Click to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

- Deactivate the check box next to the work system that you want to remove from 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.

See also

Creating a work system (chapter 5.10.3.2, page 785)

Assigning a work system to a method (chapter 5.10.3.3, page 786)

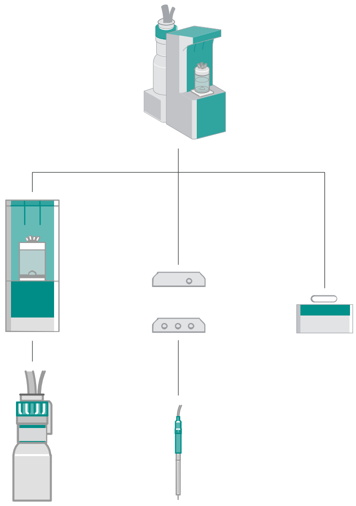
Method – Properties (chapter 5.9.2.2, page 283)

5.10.4 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** working range. 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 5.10.4.1, page 789)

Functional unit – Status (chapter 5.10.2.2, page 705)

Functional unit – Manual control (chapter 5.10.2.5, page 708)

5.10.4.1 Additional component – Directory

- *Additional components for OMNIS instruments*
- *Additional components for Metrohm USB instruments*

Additional components for OMNIS instruments

Analog sensors

Analog sensors can be connected to a measuring module of the **Measuring Module Analog** type. The following sensor types are available: Other sensor, ion-selective electrode, metal electrode, pH electrode, polarizable metal electrode.

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: pH electrode, metal electrode and ion-selective electrode.

A measuring interface and a memory chip are installed in the sensor on which all sensor data is saved. The data extracted from the sensor chip is displayed in the properties of the sensor.

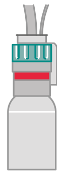
Conductivity standard

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.

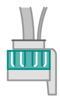
The bottle cap has a memory chip to which the solution data is saved. The solution data is read out from the attached Liquid Adapter, which transmits the data to the OMNIS Software. The properties of the solution can be edited and stored on the memory chip.



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.

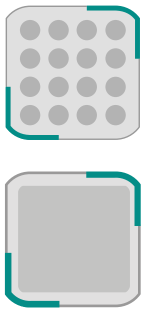
The bottle cap contains a memory chip containing information (such as solution name, concentration, concentration unit, etc.) which is defined by the manufacturer and cannot be changed. Other properties of the solution (e.g. titer, titer unit) can be edited. The information on the memory chip is read 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 beakers and is placed on the rack base of the **OMNIS Sample Robot**. The detection by the sample robot is confirmed with a beep sound and the sample rack is displayed automatically in the overview of the instrument and in the overview list of the sample rack. The sample rack is available for various beaker sizes.

In the overview of the instrument, the sample rack with the corresponding number of positions for sample beakers 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

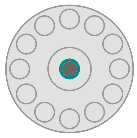
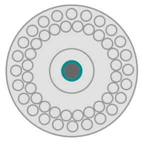
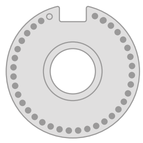
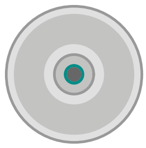
Analog sensors can be connected to a measuring interface of the **Measuring interface analog**, **Measuring interface conductivity** or **Interface coulometry** type. The following sensor types are available: Other sensor, ion-selective electrode, conductivity measuring cell, metal electrode, pH electrode, polarizable metal electrode, temperature sensor.

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.

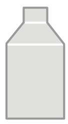





Sample processor rack

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 rack 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 sample vessels of various 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

Solution – Definition (chapter 5.10.6, page 818)

Solution – Status (chapter 5.10.6.2, page 825)

Sample rack – Definition (chapter 5.10.7, page 830)

Sample rack – Status (chapter 5.10.7.2, page 837)

Sensor – Definition (chapter 5.10.5, page 794)

Sensor – Status (chapter 5.10.5.3, page 802)

5.10.5 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.

NOTICE

Additional information regarding the various product types: *Additional component – Directory (see chapter 5.10.4.1, page 789)*

Overview list

NOTICE

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**.

The following information is displayed by default in the overview list of the sensors:

	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	Name of the **Measuring Module**, **Measuring interface** or **Interface coulometry** to which the sensor is currently connected.
Calibration date	Date of the last calibration of the sensor of the **pH electrode**, **Ion-selective electrode** or **Conductivity measuring cell** type.
Calibration expiry date	Expiry date of the calibration validity of the sensor of the **pH electrode**, **Ion-selective electrode** or **Conductivity measuring cell** type. The monitoring status of the calibration is displayed with an icon that varies in accordance with status.
Sensor expiry date	Expiry date of the working life of the sensor. The monitoring status of the sensor is displayed with an icon that differs based on status.

See also

Ion-selective electrode – Calibrating (chapter 5.10.5.5, page 805)

pH electrode – Calibrating (chapter 5.10.5.4, page 803)

Sensor – Status (chapter 5.10.5.3, page 802)

Activating sensor monitoring (chapter 5.10.5.9, page 813)

OMNIS Software – Inventory (chapter 5.2.2, page 99)

5.10.5.1 Assigning the conductivity measuring cell

You use the assignment to define with which conductivity measuring cells the individual commands will be carried out within methods.

To be able to assign conductivity measuring cells to a command, these sensors must be included in the sensor list. Furthermore, a work system that contains a functional unit of the **Measuring interface conductivity** type must be assigned to the method.

Assigning the Measuring interface conductivity and the conductivity measuring cell

Prerequisites:

- The conductivity measuring cells that are available are listed in the **Sensors** subsection in the **Equipment** work area.
- A work system with a **Measuring interface conductivity** is assigned to the method.
- The method is opened.
  To assign the conductivity measuring cell to a command, proceed as follows:

1 Selecting the command

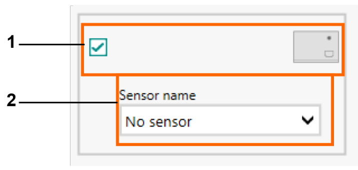
- Select the desired command in the method.

2 Opening the 'Execute with' subsection

- Click to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

3 Assigning the Measuring interface conductivity

- Activate the check box (**1**) for the desired **Measuring interface conductivity**.



The drop-down list with the names of the available conductivity measuring cells (**2**) is displayed.

NOTICE

An error message will appear if **No sensor** is selected for the sensor while a method is being run or if the selected conductivity measuring cell is no longer present in the sensor list.

4 Selecting the conductivity measuring cell

- Select a conductivity measuring cell from the drop-down list (**2**).

5 Saving changes

- Save changes by clicking on .

Removing the assignment of the Measuring interface conductivity

1 Selecting the command

- Select the desired command in the method.

2 Opening the 'Execute with' subsection

- Click to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

3 Removing the assignment

- Deactivate the check box (**1**) for the **Measuring interface conductivity**.

4 Saving changes

- Save changes by clicking on .

See also

Sensor – Definition (chapter 5.10.5, page 794)

Sensor – Status (chapter 5.10.5.3, page 802)

MEAS COND – Properties (chapter 5.9.4.12.1.1, page 467)

5.10.5.2 Sensor – Properties

Clicking on [icon] 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**.

NOTICE

- To change the properties of a digital sensor of the dTrode type or of an intelligent sensor of the iTrode type, 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.
Serial number	Display the serial number of the sensor.

Specific data

The **Sensor data** parameter group is displayed for all digital, intelligent and analog sensors.

Sensor data	
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, use the date selection 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. *Sensor – Status (see chapter 5.10.5.3, page 802)*
Comment	Enter a comment (optional). Comment length: max. 250 characters.
Ion (only ISE)	Select the ion for which the concentration is to be determined with the electrode.
Ion charge (only ISE)	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-.

The **Temperature sensor** parameter group is displayed for the following sensors:

- All digital and intelligent sensors of the pH electrode and ion-selective electrode types.
- All analog sensors of the analog pH electrode and ion-selective electrode types.
- Conductivity measuring cells.

Temperature sensor	
Type of temperature sensor	Display the type of the temperature sensor.
R (25 °C) (only digital pH electrode)	With temperature sensors of the NTC-B type, the nominal resistance value must be specified at 25 °C (R(25 °C)).
B value (only digital pH electrode)	The thermistor constant (B value) must be specified for temperature sensors of the NTC-B type. The thermistor constant is a material constant.

The **Reference electrode** parameter group is displayed for all digital sensors of the dTrode type as well as for analog ion-selective electrodes and analog metal electrodes.

Reference electrode	
Article number (only analog metal electrode and analog ISE)	Display or enter the number that unambiguously identifies the reference electrode.
Serial number (only analog metal electrode and analog ISE)	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 intermediate electrolyte type (aqueous, nonaqueous, gel, not available).
Bridge electrolyte	Enter the electrolyte that is used between the reference electrode and the measuring electrode.

The **Calibration data** parameter group is displayed for all ion-selective electrodes (ISE), conductivity measuring cells and pH electrodes.

Calibration data	
Slope	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 ISE)	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 ISE)	Enter the blank value concentration c(blank). The concentration of a blank is subtracted from the analysis result.
Unit (only ISE)	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	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	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	Temperature of the first calibration buffer, which was measured with a temperature sensor during the calibration.
Temperature sensor	Display the temperature sensor 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.

Calibration data	
Calibration date	Display the date on which the calibration was carried out.
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. *Sensor – Status (see chapter 5.10.5.3, page 802)*
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.

The **Connection** parameter group is displayed for all digital and intelligent sensors.

Connection	
Connected to	Display the measuring module or the measuring interface to which the sensor is connected.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Sensor – Definition (chapter 5.10.5, page 794)

Sensor – Status (chapter 5.10.5.3, page 802)

OMNIS Software – Inventory (chapter 5.2.2, page 99)

5.10.5.3 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

Activating sensor monitoring (chapter 5.10.5.9, page 813)

Sensor – Properties (chapter 5.10.5.2, page 798)

5.10.5.4 pH electrode – Calibrating

General notes

Assigning the sensor

pH electrodes can be calibrated with the **CAL pH** 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.

Calibration temperature

For an accurate calibration result, the temperature of all the calibration buffers used must be kept **constant** during the calibration. 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 put in manually in the **CAL pH** command in the corresponding input field in the **Parameters** subsection of the **Properties** window.

Recognizing calibration buffers automatically

On the basis of the measured potential, the correct buffer for the selected buffer type and the appropriate buffer value for the calibration temperature are recognized. If the same buffer is recognized for the first and second calibration solution, the calibration is canceled with an error message.

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.

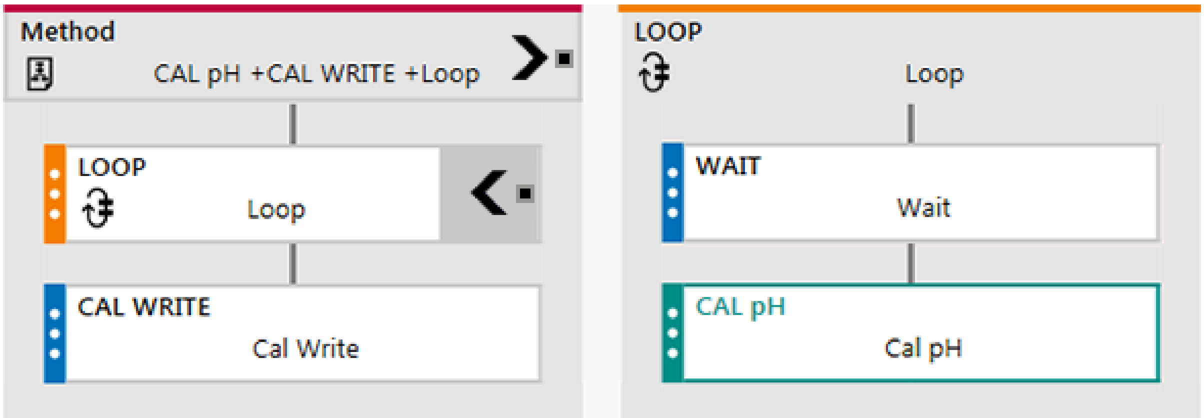


Figure 7 Example method of a calibration with a subsample using the LOOP command.

- 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.
- Make sure that the number of loop passes 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 the calibration without automation, the **WAIT** command is used to interrupt the method run with each loop pass so that the calibration buffers can be replaced manually. The message defined in the **WAIT** command must be confirmed to continue the method run.
- For the calibration with automation (e.g. with an **OMNIS Sample Robot**), the beakers with the buffer solutions must be placed on the same sample rack consecutively.

- We recommend using the provided operating procedure templates for the calibration with automation (e.g. with an **OMNIS Sample Robot**). (See: *Importing the templates (see 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.

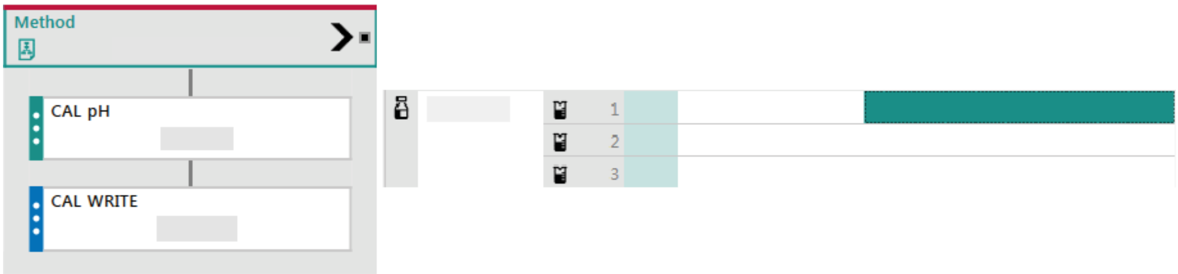


Figure 8 Example method of a calibration with multiple subsamples.

- 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.
- We recommend using the provided operating procedure templates for the calibration with automation (e.g. with an **OMNIS Sample Robot**). (See: *Importing the templates (see chapter 3.2, page 11)*)

5.10.5.5 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.

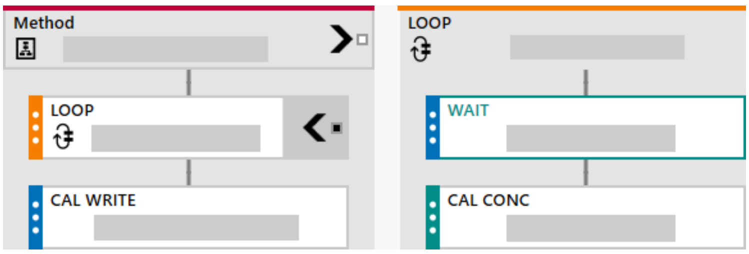
Creating samples and subsamples

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.

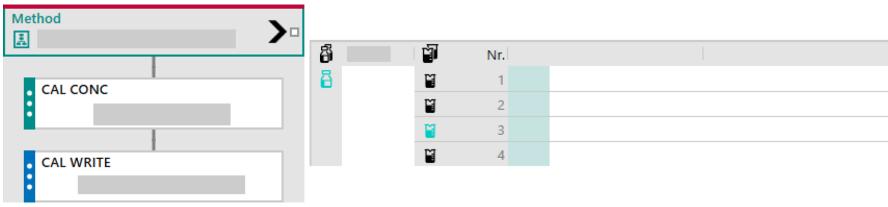


- The method contains, among others, the **LOOP**, **CAL CONC** and **CAL WRITE** commands.
- The **CAL CONC** command is in a loop and is executed according to the number of standards.
- The number of loop passes in the **LOOP** command must correspond to the defined number of calibration standards 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.

5.10.5.6 Assigning analog sensors (Metrohm USB device)

Assigning analog sensors defines with which analog sensor the titration command or measuring command is executed.

If the electrode has no in-built temperature sensor, the external temperature sensor must be connected to the temperature port of the same analog measuring interface.

Assigning the measuring interface and analog sensors

Prerequisites:

- The required analog sensors were added to the sensor list in **Equipment ▶ Sensors**.
- A work system with an analog measuring interface is assigned to the method.
- The method is opened.

1 Selecting the command

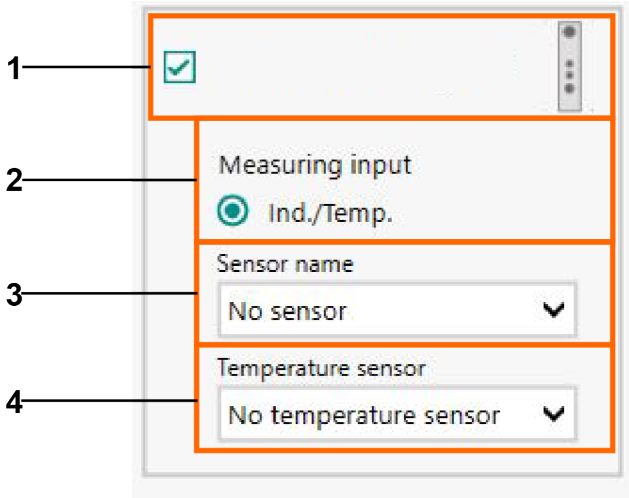
- Select the desired command in the method.

2 Opening the 'Execute with' subsection

- Click on to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

3 Assigning the analog measuring interface

- Activate the check box (1) for the desired measuring module.



The measuring input (2) is selected automatically.

NOTICE

An error message appears if the selected sensor is no longer in the sensor list or if it is listed several times while a method is being run.

If **No sensor** is selected when a method is being executed, the determination is executed without an error message.

4 Selecting a sensor

- Select the sensor from the selection list (3).

5 Selecting a temperature sensor

- If a temperature measurement is carried out with a separate temperature sensor, select the temperature sensor or pH electrode with integrated temperature sensor in the selection list (4).

6 Saving changes

- Save changes by clicking on 🖫.

Removing the assignment of the analog measuring interface

1 Selecting the command

- Select the desired command in the method.

2 Opening the 'Execute with' subsection

- Click on ⚙ to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

3 Removing the assignment

- Deactivate the check box (1) for the analog measuring interface.

4 Saving changes

- Save changes by clicking on 🖫.

See also

Sensor – Definition (chapter 5.10.5, page 794)

Sensor – Status (chapter 5.10.5.3, page 802)

5.10.5.7 Assigning digital sensors

You use the assignment to define with which digital measuring module the individual commands will be carried out within methods. The digital sensor connected to the measuring module is used for the measurement. The calibration data is saved to the sensor.

For a digital sensor to be able to be assigned to a command, a work system that contains a digital measuring module must be assigned to the method.

Assigning a digital measuring module

Prerequisites:

- A work system with a digital measuring module is assigned to the method.

- The method is opened.
To assign the digital measuring module to a command, proceed as follows:

1 Selecting the command

- Select the symbol of the desired command in the method.

2 Selecting the 'Execute with' subsection

- Click on to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

3 Assigning a digital measuring module

- Activate the check box for the desired measuring module.

4 Saving changes

- Save changes by clicking on .

Removing the assignment of a digital measuring module

1 Selecting the command

- Select the symbol of the desired command in the method.

2 Selecting the 'Execute with' subsection

- Click on to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

3 Removing the assignment

- Deactivate the check box for the digital measuring module.

4 Saving changes

- Save changes by clicking on .

5.10.5.8 Assigning analog sensors

Assigning analog sensors defines with which analog sensor the titration command or measuring command is executed.

If a separate temperature sensor is used at the second measuring input, it can be chosen in the sensor list and the corresponding measuring input can be selected.

Assigning the analog measuring module and analog sensors

Prerequisites:

- The required analog sensors were added to the sensor list in **Equipment ▶ Sensors**.
- A work system with an analog measuring module is assigned to the method.
- The method is opened.

1 Selecting the command

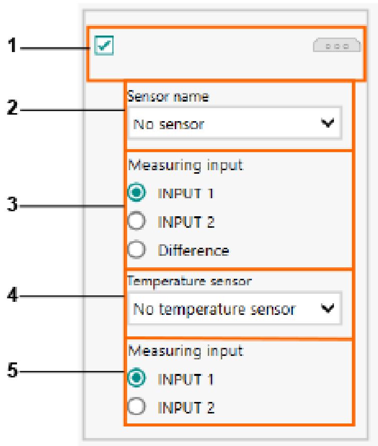
- Select the desired command in the method.

2 Opening the 'Execute with' subsection

- Click on to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

3 Assigning the analog measuring module

- Activate the check box (**1**) for the desired measuring module.



The selection list with the sensor names (**2**) and the selection of the measuring inputs (**3**) are displayed.

NOTICE

An error message appears if the selected sensor is no longer in the sensor list or if it is listed several times while a method is being run.

If **No sensor** is selected when a method is being executed, the determination is executed without an error message.

4 Selecting a sensor

- Select the sensor from the selection list (**2**).

5 Selecting the measuring input

- Select the measuring input **INPUT 1**, **INPUT 2** or **Difference** (**3**) at the measuring module.

NOTICE

- For a combined pH electrode with integrated temperature sensor, the same **INPUT** must be selected for both measuring inputs.
- If the measuring input cannot be selected, the selection option for the measuring input (**3** and **5**) is not active.

6 Selecting a temperature sensor

- If a temperature measurement is carried out with a separate temperature sensor, select the temperature sensor or pH electrode with integrated temperature sensor from the selection list (**4**).

NOTICE

If **Difference** is selected as measuring input, no temperature sensor can be selected.

7 Selecting a measuring input for temperature measurements

- Select the measuring input **INPUT 1** or **INPUT 2** (**5**) for the temperature sensor.

NOTICE

For all **Ipol** commands, the temperature sensor is fixed at **INPUT 2**, as it is mandatory that the polarizable metal electrode is connected to **INPUT 1**.

8 Saving changes

- Save changes by clicking on .

Removing the assignment of the analog measuring module

1 Selecting the command

- Select the desired command in the method.

2 Opening the 'Execute with' subsection

- Click on to open the **Properties** window.
- In the **Properties** window, select the **Execute with** subsection.

3 Removing the assignment

- Deactivate the check box (**1**) for the analog measuring module.

4 Saving changes

- Save changes by clicking on .

See also

Sensor – Definition (chapter 5.10.5, page 794)

Sensor – Status (chapter 5.10.5.3, page 802)

5.10.5.9 Activating sensor monitoring

The OMNIS Software can be used to execute the following actions for the monitoring of a sensor:

- *(see "Monitoring the sensor data", page 814)*
  This function is needed to monitor the **Working life** and the **Expiry date** of a sensor.
- *(see "Monitoring the calibration data", page 815)*
  This function is needed to monitor the **Validity period** and the **Expiry date** of the calibration of a sensor.

- *(see "Defining the Advance warning time", page 816)*
  This function is needed to define when the user is to be warned before the working life of a sensor expires.

NOTICE

If the **Working life** or the **Calibration validity** expires during the determination of a subsample, 2 options are available: *(see "Carrying out a determination after the expiry date is reached", page 816)*.

Monitoring the sensor data

Prerequisite:

- The sensor to be monitored is selected in **Equipment ▶ Sensors**.

1 Opening the Properties window

- Click on to open the **Properties** window.

2 Entering the working life of the sensor

- Enter the working life of the sensor in days in **Specific data ▶ Sensor data**.
  or
- Click on to select a date which sets the working life of the sensor.

3 Activating sensor monitoring

- Activate the **Enable monitoring** function by clicking on the check box.

Once monitoring is activated, then the monitoring status is displayed in the respective column in the overview list of the sensors *Sensor – Status (see chapter 5.10.5.3, page 802)*.

4 Saving changes

- Save changes by clicking on .

NOTICE

- Modified data of a digital or intelligent sensor cannot be saved as long as the sensor is being used in a running determination.
- The basis for the calculation of an expiry date or time interval are the date and time settings of the operating system used, i.e. time zones, summer time and leap years are taken into account.
- If the date and time settings are changed, the expiry dates, calibration data and working life initially entered will not be changed. These dates are saved on the sensors as well as in the database.

Monitoring the calibration data

NOTICE

This function is only available for sensors of the types ion-selective electrode, conductivity measuring cell and ph electrode.

Prerequisite:

- The sensor for which the calibration is to be monitored is selected in **Equipment ▶ Sensors**.

1 Opening the Properties window

- Click on to open the **Properties** window.

2 Entering the validity period of the sensor calibration

- Enter the validity period of the sensor calibration in hours in **Specific data ▶ Calibration data**.

3 Activating the monitoring of the sensor calibration

- Activate the **Enable monitoring** function by clicking on the check box.

Once monitoring is activated, then the monitoring status is displayed in the respective column in the overview list of the sensors *Sensor – Status (see chapter 5.10.5.3, page 802)*.

4 Saving changes

- Save changes by clicking on .

Defining the Advance warning time

NOTICE

- Optionally, an **Advance warning time** can be defined for the **Working life** of every sensor type. The replacement of sensors can be planned on time as a result.
- No **Advance warning time** can be defined for the **Validity period** of the sensor calibration.

Prerequisite:

- The sensor overview under **Equipment ▶ Sensors** is open.

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 sensor type. In order for the advance warning time defined here to be applied, *(see "", page 814)* must be activated for at least one sensor of the relevant sensor type.
- Enter the required **Advance warning time** in days.

NOTICE

If no advance warning time is to be defined for a sensor type, the **No advance warning** option (default value) must be selected in the selection list.

3 Saving the advance warning time

- Save changes by clicking on .

Once the time for which the advance warning time is set has been reached, a warning appears. 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

A warning appears if a determination is to be carried out with a sensor for which the expiry date has elapsed. To execute the determination, the following options are available:

- *(see "Canceling and restarting the determination", page 817)*
- *(see "Continuing the determination", page 817)*

NOTICE

If a method contains a command of the types **CAL pH**, **CAL CONC** or **CAL COND**, no warning is displayed for a sensor for which the calibration has expired. The sensor is re-calibrated when the commands mentioned are used.

Canceling and restarting the determination

Prerequisite:

- A determination was started in the **Sample list**.
- The **Working life** or the **Calibration validity** of a sensor has expired or has been exceeded.
- Before the determination of the subsample is executed, the warning **Expiry date exceeded** is displayed.

1 Canceling the determination

- Click on **[Cancel]** in the warning message to cancel the execution of the subsample.
- Replace the sensor or re-calibrate it.

The status of the subsample is reset to **Ready** automatically.

NOTICE

The determination can be continued despite the **Working life** or **Calibration validity** of a sensor having expired. Click on **[Continue]** in the warning message to continue the execution of the subsample.

2 Restarting the determination

- Start the determination of the subsample again by clicking on ▶.

Continuing the determination

Prerequisite:

- A determination was started in the **Sample list**.

- The **Working life** or the **Calibration validity** of a sensor has expired or has been exceeded.
- Before the determination of the subsample is executed, the warning **Expiry date exceeded** is displayed.

1 Continuing the determination

- Click on **[Continue]** in the warning message to continue the execution of the subsample despite the **Working life** or the **Calibration validity** of a sensor having expired.

NOTICE

If the determination is executed with a sensor for which the **Working life** or the **Calibration validity** has expired, the measuring results may be flawed.

See also

Sensor – Definition (chapter 5.10.5, page 794)

Sensor – Status (chapter 5.10.5.3, page 802)

5.10.6 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.

NOTICE

Additional information regarding the various solution types: *Additional component – Directory (see chapter 5.10.4.1, page 789)*

Overview list

NOTICE

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.

The following information is displayed by default in the overview list of the solutions:

	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.

See also

Solution – Properties (chapter 5.10.6.1, page 819)

Solution – Status (chapter 5.10.6.2, page 825)

Creating a Conductivity table (chapter 5.10.9, page 859)

5.10.6.1 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	
Solution 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.
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.

Solution data	
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 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.

Solution data	
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**.

NOTICE

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.
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.

Connection	
Connected to	Display the dosing unit to which the solution is connected.

> **NOTICE**
>
> - 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

> **NOTICE**
>
> 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

User rights – Directory (chapter 4.6.7.3, page 62)

Solution – Status (chapter 5.10.6.2, page 825)

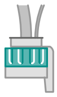
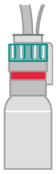
Activating solution monitoring (chapter 5.10.6.3, page 826)

Creating a Conductivity table (chapter 5.10.9, page 859)

Sensor – Status (chapter 5.10.5.3, page 802)

5.10.6.2 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

Solution – Definition (chapter 5.10.6, page 818)

Activating solution monitoring (chapter 5.10.6.3, page 826)

Solution – Properties (chapter 5.10.6.1, page 819)

User rights – Directory (chapter 4.6.7.3, page 62)

5.10.6.3 Activating solution monitoring

The OMNIS Software can be used to execute the following actions for the monitoring of a solution:

- *(see "Monitoring the expiry date of titers and solutions", page 826)*
  This function is needed to monitor the **Working life** and the **Expiry date** of a solution or a titer.
- *(see "Defining the Advance warning time", page 827)*
  This function is needed to define when the user is to be warned before the working life of a solution expires.

NOTICE

If the **Working life** expires during the determination of a subsample, 2 options are available: *(see "Carrying out a determination after the expiry date is reached", page 828)*.

Monitoring the expiry date of titers and solutions

Prerequisite:

- The user has the **Manage solutions** right.
- The solution to be monitored is selected in **Equipment ▶ Solutions**.

1 Opening the Properties window

- Click on to open the **Properties** window.

2 Enter the working life of the solution

- Enter the working life of the solution in days in **Specific data ▶ Solution data**.
  or
- Click on 15 to select a date which sets the working life of the solution.

3 Activating the solution monitoring

- Activate the **Enable monitoring** function by clicking on the check box.

Once monitoring is activated, then the monitoring status is displayed in the respective column in the overview list of the solutions *Solution – Status* *(see chapter 5.10.6.2, page 825)*.

4 Entering the validity period of the titer

- Enter the validity period of the titer in days in **Specific data ▶ Titer data**.
  or
- Click on 15 to select a date which sets the validity period of the titer.

5 Activating titer monitoring

- Activate the **Enable monitoring** function by clicking on the check box.

Once monitoring is activated, then the monitoring status is displayed in the respective column in the overview list of the solutions *Solution – Status* *(see chapter 5.10.6.2, page 825)*.

6 Saving changes

- Save changes by clicking on .

NOTICE

- Modified data of a solution cannot be saved as long as the solution is being used in a running determination.
- The basis for the calculation of an expiry date or time interval are the date and time settings of the operating system used, i.e. time zones, summer time and leap years are taken into account.
- If the date and time settings are changed, the expiry dates, adsorber data and working life initially entered will not be changed. This data is saved on the solutions as well as in the database.

Defining the Advance warning time

Optionally, an **Advance warning time** can be defined for the **Working life** of a solution and the **Validity period** of a titer. The replacement of solutions can be planned on time as a result.

Prerequisite:

- The user has the **Manage solutions** right.

- The **Equipment ▶ Solutions** subsection is opened.

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 the data that is to be monitored. In order for the advance warning time defined here to be applied, *(see "", page 826)* must be activated for at least one solution.
- Enter the required **Advance warning time** in days.

NOTICE

If no advance warning time is to be defined for **Solution data** or **Titer data**, the **No advance warning** option (default value) must be selected in the selection list.

3 Saving the advance warning time

- Save changes by clicking on .

Once the time for which the advance warning time is set has been reached, a warning appears. 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

A warning appears if a determination is to be carried out with a solution for which the expiry date has elapsed. To execute the determination, the following options are available:

- *(see "Canceling and restarting the determination", page 828)*
- *(see "Continuing the determination", page 829)*

Canceling and restarting the determination

Prerequisite:

- A determination was started in the **Sample list**.
- The **Working life** of a solution or the **Validity period** of a titer has expired or has been exceeded.
- Before the determination of the subsample is executed, the warning **Expiry date exceeded** is displayed.

- The user has the **Manage solutions** right.

1 Canceling the determination

- Click on **[Cancel]** in the warning message to cancel the execution of the subsample.
- Replace the solution.

The status of the subsample is reset to **Ready** automatically.

2 Restarting the determination

- Start the determination of the subsample again by clicking on ▶.

Continuing the determination

Prerequisite:

- A determination was started in the **Sample list**.
- The **Working life** of a solution or the **Validity period** of a titer has expired or has been exceeded.
- Before the determination of the subsample is executed, the warning **Expiry date exceeded** is displayed.

1 Continuing the determination

- Click on **[Continue]** in the warning message to continue the execution of the subsample despite the working life or the titer validity of a solution having expired.

NOTICE

If the determination is executed with a solution for which the working life or the titer validity has expired, the measuring results may be flawed.

See also

Solution – Definition (chapter 5.10.6, page 818)

Sensor – Status (chapter 5.10.5.3, page 802)

5.10.7 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.

NOTICE

Additional information regarding the various sample rack types: *Additional component – Directory (see chapter 5.10.4.1, page 789)*

All recognized sample racks are displayed in an overview list under **Equipment ▶ Sample racks**.

Overview list

NOTICE

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.

The following information is displayed by default in the overview list of the sample racks:

	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	English designation of the product.

Name	Name of the sample rack that can be adapted in the **Properties** of the sample rack.
Placed on	Name of the sample robot or sample changer on whose rack base or turntable the sample rack is placed.
Position	Number of the rack position (RP1 – RP7)
Number of positions	Number of positions on the sample rack.

See also

Sample rack – Status (chapter 5.10.7.2, page 837)

Sample rack – Properties (chapter 5.10.7.1, page 831)

5.10.7.1 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**:

NOTICE

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: *Importing rack parameters (see chapter 5.10.7.4, page 839)*

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: *Exporting rack parameters (see chapter 5.10.7.5, page 840)*

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 with the order 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.
Beaker diameter (only OMNIS sample rack)	Display the diameter (in mm) of the sample beaker.
Beaker height (only OMNIS sample rack)	Display the height (in mm) of the sample beaker.
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.

Rack data	
Vessel sensor (only Sample processor rack of 874 Oven Sample Processor)	Select or deactivate the 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 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**: Deactivate 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 sample robot or sample changer on which rack base or turntable the sample rack is mounted.

Positions on the rack

NOTICE

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**.

NOTICE

For the 1-tower version of sample changers, the values of the **Tower 1** parameter group are used.

Sample positions	
Vessel sensor	Select or deactivate the 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 sample vessel is present at the selected position: ▪ **Tower**: Activate the vessel sensor installed in the tower. Only positions on single-row 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. ***Note***: This vessel sensor selection only applies for sample positions. The vessel sensor can be specifically selected or deactivated for each special position. ***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.

Tower 1–2	
Work height	Enter the height (in mm) that the lift moves 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 *Defining the lift height (see chapter 5.10.2.43, page 774)*.

Tower 1–2	
Rinse height	Enter the height (in mm) that the lift moves 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 *Defining the lift height (see chapter 5.10.2.43, page 774)*.
Change height	Enter the height (in mm) that the lift moves 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 *Defining the lift height (see chapter 5.10.2.43, page 774)*.
Special height	Enter the user-defined height (in mm) that can be used e.g. to immerse a pipetting tip. ***Note***: The special height only applies for positions on the rack.

A **special position** can be added by clicking :*Defining a special position (see chapter 5.10.2.44, page 778)*

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.

Special position	
Vessel sensor	Select or deactivate 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 deactivated in the same subsection in the **Sample positions** parameter group. ***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.

Tower 1–2	
Work height	Enter the work height (in mm) that the lift is moved 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.

NOTICE

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

User rights – Directory (chapter 4.6.7.3, page 62)

Defining the lift height (chapter 5.10.2.43, page 774)

Sample rack – Definition (chapter 5.10.7, page 830)

Sample rack – Status (chapter 5.10.7.2, page 837)

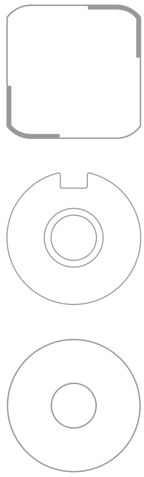
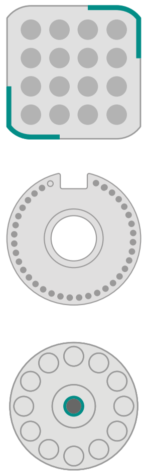
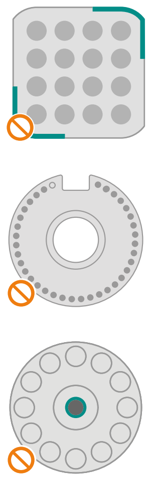
Exporting rack parameters (chapter 5.10.7.5, page 840)

Importing rack parameters (chapter 5.10.7.4, page 839)

Defining a special position (chapter 5.10.2.44, page 778)

5.10.7.2 Sample rack – Status

The status of the sample racks is represented in the **Instruments** subsection as follows:

	**OMNIS Sample Robot**: No sample rack has been placed on the rack base. **Sample Processor**: No sample rack has been placed on the turntable or the magnet code of the mounted sample rack has not been read yet by initializing the sample changer.
	**OMNIS Sample Robot**: A sample rack has been placed on the rack base. The name of the sample rack is displayed in the tooltip. **Sample Processor**: A sample rack has been placed on the turntable. The name of the sample rack is displayed in the tooltip.
	**OMNIS Sample Robot**: A sample rack has been placed on the rack base. Samples of this sample rack are currently being used in the determination run. **Sample Processor**: A sample rack has been placed on the turntable. Samples of this sample rack are currently being used in the determination run.

NOTICE

For OMNIS sample racks: A sample rack that is used in the determination run must not be removed from the rack base. One or more samples may be in progress and must be placed back onto the sample rack.

For Sample Processor racks: A sample rack that is used in the determination run must not be removed from the turntable.

5.10.7.3 Importing a rack definition

In order for a customized sample rack to be used by the OMNIS Software, its rack definition must be imported into the OMNIS Software. After importing the rack definition, placing the sample rack on the sample changer and initializing the instrument according to these instructions, the sample rack appears in the **Sample racks** subsection.

Prerequisite:

- The rack definition to be imported is available as XML file.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Importing a rack definition

- Click on to open the **Import rack definition** Explorer window under **Equipment ▶ Sample racks**.

2 Browsing for folder

- Select the folder in which the import file is saved.

3 Selecting the file type

- Select the *.xml file type at the bottom right of the Explorer window.
- Select the import file or enter the name of the import file in the **File name** field.

4 Confirming and importing the selection

- Click on **[Open]** to confirm the selection.

The rack definition is imported into the OMNIS Software. After placing the sample rack on the sample changer and initializing the instrument, the sample rack appears in the **Sample racks** subsection.

NOTICE

If the rack code of the rack definition to be imported is invalid or already exists in a rack definition in the OMNIS Software, the **Rack code invalid or already exists** dialog opens. The rack name and the rack code for the sample rack can be newly defined in the dialog.

NOTICE

The customized sample rack is not recognized automatically by the OMNIS Software when reserving the sample changer. In order for the sample rack 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 – Properties (chapter 5.10.7.1, page 831)

5.10.7.4 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.
- The OMNIS rack configuration file (*.orco) is available.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Importing 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 **Import rack parameters** explorer window by clicking on [icon] in the **Properties** window.

NOTICE

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 import file is saved.

3 Selecting the file type

- Select the required OMNIS rack configuration file (.orco) or enter the name of the import file in the **File name** field.

4 Confirming and importing the selection

- Click on **[Open]** to confirm the selection.

The rack parameters for the selected sample rack are imported into the OMNIS Software.

See also

Sample rack – Properties (chapter 5.10.7.1, page 831)

Exporting rack parameters (chapter 5.10.7.5, page 840)

5.10.7.5 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. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

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** explorer window by clicking on in the **Properties** window.

NOTICE

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 that the exported file is to be saved in.

3 Defining a file name (optional)

- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

4 Creating an export file

- Click on **[Save]**, to create the export file.

The rack parameters are exported as a file to the selected folder.

NOTICE

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**.

See also

Sample rack – Properties (chapter 5.10.7.1, page 831)

Importing rack parameters (chapter 5.10.7.4, page 839)

5.10.8 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

CAL pH – Properties (chapter 5.9.4.13.1, page 504)

pH electrode – Calibrating (chapter 5.10.5.4, page 803)

Metrohm buffer type (chapter 5.10.8.2, page 845)
Metrohm buffer type (chapter 5.10.8.2, page 845)

Baker buffer type (chapter 5.10.8.3, page 846)

Beckmann buffer type (chapter 5.10.8.4, page 847)

DIN buffer type (in accordance with DIN standard 19267, 2012) (chapter 5.10.8.5, page 848)

Fisher buffer type (chapter 5.10.8.6, page 849)

Fluka buffer type (chapter 5.10.8.7, page 851)

Hamilton DURACAL buffer type (chapter 5.10.8.8, page 852)

Merck CertiPUR 20/Titrisol buffer type (chapter 5.10.8.9, page 853)

Buffer type Merck CertiPUR 25 (chapter 5.10.8.10, page 854)

Mettler Toledo buffer type (chapter 5.10.8.11, page 855)

NIST buffer type (chapter 5.10.8.12, page 856)

Radiometer Analytical buffer type (chapter 5.10.8.13, page 858)

Editing custom calibration buffers (chapter 5.10.8.1, page 843)

5.10.8.1 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, empty temperature tables for 2 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 empty temperature tables for 2 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).

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.

NOTICE

For custom calibration buffers enter at least the pH values for the temperature range in which your pH calibration and pH measurement will later be carried out.

See also

Calibration buffers – Definition (chapter 5.10.8, page 842)

Metrohm buffer type (chapter 5.10.8.2, page 845)

Metrohm buffer type (chapter 5.10.8.2, page 845)

Baker buffer type (chapter 5.10.8.3, page 846)

Beckmann buffer type (chapter 5.10.8.4, page 847)

DIN buffer type (in accordance with DIN standard 19267, 2012) (chapter 5.10.8.5, page 848)

Fisher buffer type (chapter 5.10.8.6, page 849)

Fluka buffer type (chapter 5.10.8.7, page 851)

Hamilton DURACAL buffer type (chapter 5.10.8.8, page 852)

Merck CertiPUR 20/Titrisol buffer type (chapter 5.10.8.9, page 853)

Buffer type Merck CertiPUR 25 (chapter 5.10.8.10, page 854)

Mettler Toledo buffer type (chapter 5.10.8.11, page 855)

NIST buffer type (chapter 5.10.8.12, page 856)

Radiometer Analytical buffer type (chapter 5.10.8.13, page 858)

5.10.8.2 Metrohm buffer type

NOTICE

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

NOTICE

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.

5.10.8.3 Baker buffer type

NOTICE

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

Temp. (°C)	pH 4.00	pH 7.00	pH 9.00	pH 10.00
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	-	-	-	-

NOTICE

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.

5.10.8.4 Beckmann buffer type

NOTICE

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

Temp. (°C)	**pH 4.000**	**pH 7.000**	**pH 10.010**
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	-

NOTICE

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.

5.10.8.5 DIN buffer type (in accordance with DIN standard 19267, 2012)

NOTICE

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*

Temp. (°C)	pH 1.09	pH 3.06	pH 4.65	pH 6.79	pH 9.23	pH 12.75
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	-	-	-	-	-	-

NOTICE

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.

5.10.8.6 Fisher buffer type

NOTICE

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*

NOTICE

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.

5.10.8.7 Fluka buffer type

NOTICE

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*

NOTICE

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.

5.10.8.8 Hamilton DURACAL buffer type

NOTICE

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	-	-	-	-

Temp. (°C)	pH 4.01	pH 7.00	pH 9.21	pH 10.01
90	-	-	-	-
95	-	-	-	-

NOTICE

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.

5.10.8.9 Merck CertiPUR 20/Titrisol buffer type

NOTICE

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

Temp. (°C)	pH 2.000	pH 4.000	pH 7.000	pH 9.000	pH 12.000
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*	-	-

NOTICE

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.

5.10.8.10 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

Temp. (°C)	pH 4.00	pH 7.00	pH 9.00	pH 10.00
55	-	-	-	-
60	-	-	-	-
65	-	-	-	-
70	-	-	-	-
75	-	-	-	-
80	-	-	-	-
85	-	-	-	-
90	-	-	-	-
95	-	-	-	-

NOTICE

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.

5.10.8.11 Mettler Toledo buffer type

NOTICE

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

Temp. (°C)	pH 2.00	pH 4.01	pH 7.00	pH 9.21	pH 11.00
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*	-

NOTICE

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.

5.10.8.12 NIST buffer type

NOTICE

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	-

NOTICE

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.

5.10.8.13 Radiometer Analytical buffer type

NOTICE

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
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	-	-	-	-

NOTICE

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.

5.10.9 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: *User rights – Directory (see chapter 4.6.7.3, page 62)*

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.

NOTICE

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.

NOTICE

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

Assigning the conductivity measuring cell (chapter 5.10.5.1, page 796)

CAL COND – Properties (chapter 5.9.4.13.3, page 521)

5.10.10 Standards – Subsection

The following functions are available in **Equipment ▶ Standards**:

- Use **Import standards** to import data of a standard from an OMNIS standard file.
- Use **Save** to save all changes.
- ✗ Use **Delete standards** to delete the standard. If the standard was used in another method, than another valid standard must be selected in the command parameters.

Definition

The term **Standards** is used in the OMNIS Software for **NIR reflection standards**. NIR reflection standards are used for reference standardization and for testing the signal noise.

Standards can be imported as an **OMNIS standard file** (*.ostd).

The **Reflection** and **Transmission** measuring modes are available in the command parameters of the **REF STD** command, the **VAL REF STD** command and the **TEST NOISE** command. NIR reflection standards are required for the reference standardization, the validation and the testing of the signal noise in **reflection mode**.

To use a standard in the OMNIS Software, it must first be imported: *Importing standards (see chapter 5.10.10.2, page 862)*. The standard must be held in front of the measuring probe during reference standardization, validation or testing of the signal noise.

NOTICE

Further information on the commands: *REF STD – Properties (see chapter 5.9.4.6, page 454)*, *VAL REF STD – Properties (see chapter 5.9.4.5, page 451)*, *TEST NOISE – Properties (see chapter 5.9.4.9, page 461)*

Overview list

The following information is displayed in the overview list for the standards:

Product type	English designation of the standard.
Name	Name of the standard. The name can be adapted in the properties of the standard.
Certification date	Date on which the standard was last certified. When importing a standard into the OMNIS software, the certification date is entered in the **Specific data** of the standard and displayed in the Overview list. The standard can be recertified via the regional Metrohm representative. It can then be re-imported into the OMNIS Software. The certification date will be overwritten as a result.

See also

REF STD – Properties (chapter 5.9.4.6, page 454)

Importing standards (chapter 5.10.10.2, page 862)

Standards – Properties / Specific data (chapter 5.10.10.1, page 862)

VAL REF STD – Properties (chapter 5.9.4.5, page 451)

TEST NOISE – Properties (chapter 5.9.4.9, page 461)

5.10.10.1 Standards – Properties / Specific data

Clicking on under **Equipment ▶ Standards** opens the **Properties** window. 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

REF STD – Properties (chapter 5.9.4.6, page 454)

Importing standards (chapter 5.10.10.2, page 862)

Standards – Subsection (chapter 5.10.10, page 860)

VAL REF STD – Properties (chapter 5.9.4.5, page 451)

5.10.10.2 Importing standards

Prerequisite:

- The OMNIS standard file is available.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Importing standards

- Click on to open the **Import standard** window in **Equipment ▶ Standards**.

2 Browsing for folder

- Select the folder in which the import file is saved.

3 Selecting the file type

- Select the *.ostd file type at the bottom right of the window. The standards can only be imported one by one.
- Select the import file or enter the name of the import file in the **File name** field.

4 Confirming and importing the selection

- Click on **[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.

NOTICE

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

User rights – Directory (chapter 4.6.7.3, page 62)

Standards – Subsection (chapter 5.10.10, page 860)

Standards – Properties / Specific data (chapter 5.10.10.1, page 862)

REF STD – Properties (chapter 5.9.4.6, page 454)

VAL REF STD – Properties (chapter 5.9.4.5, page 451)

5.11 Models – Actions

You can execute the following actions in the subsections of the **Models** work area:

- In **Models ▶ Prediction models**, prediction models are developed, evaluated and published. Published prediction models can be used in the determination and reprediction of results.
- In **Models ▶ Slope/y-intercept corrections**, slope/y-intercept corrections for prediction models are created, calculated and published. Published slope/y-intercept corrections can be used in the determination and reprediction of predicted results.

See also

Editing a Prediction model (chapter 5.11.1.5, page 875)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Publishing a prediction model (chapter 5.11.1.17, page 903)

Prediction model – Tab (chapter 5.2.8, page 112)

Slope/y-intercept correction – Definition (chapter 5.11.2.7, page 915)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Slope/y-intercept correction – Tab (chapter 5.2.9, page 116)

5.11.1 Prediction model – Subsection

The following functions are available in **Models ▶ Prediction models**:

- Use **Create prediction model** to create a new prediction model. Prediction models can be developed, evaluated and published for use in the determination.
- Use **Import prediction model** to import one or multiple prediction models. Imported calibration models can be edited and used or only used, depending on their types.

- Use **Export prediction model** to export the prediction model as a file.
- Use **Create Report** to create a report of the prediction model.
- Use **Duplicate prediction model** to duplicate the prediction model under the same name.
- Use **Properties** to open the properties of the selected element.
- Use **Delete prediction model** to delete the prediction model. 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 prediction model **Type full**.
Version	Current version number of the prediction model. A new version is created automatically each time it is saved or published.
Type	Type of prediction model. ▪ **full** ▪ **light**
Last published version	Name and version number of the prediction model.
Saved	Time of the last change.

NOTICE

If a Prediction model type light is imported into the OMNIS Software for which there is no Prediction model type full in the overview list, it is displayed in the **Type** column as **light**.

See also

Editing a Prediction model (chapter 5.11.1.5, page 875)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Prediction model – Tab (chapter 5.2.8, page 112)

Report template – Directory (chapter 5.8.1.4, page 155)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

5.11.1.1 Prediction model – Definition

A **Prediction model** calculates the correlation between known constituent values of different samples and their NIR spectra. Prediction models are used to predict the constituent value of unknown samples in routine analysis. Several reference parameters can be determined simultaneously for one sample. A separate prediction model must be created for each reference parameter.

The prediction models are created and managed in **Models ▶ Prediction models**. Published prediction models can be referenced in the **PREDICT** commands to evaluate spectra.

To reevaluate results, published prediction models can be selected in **Samples ▶ Results ▶ Predictions**.

NOTICE

Further information on creating a prediction model:

Follow-up of the Prediction model (see chapter 5.11.1.2, page 867)
Follow-up of the Prediction model (see chapter 5.11.1.2, page 867)

Preparing the Prediction model (see chapter 5.11.1.3, page 869)

Prediction model navigator – Functional description (see chapter 5.11.1.6, page 883)

Prediction model type full and light

The following prediction model types are available in the OMNIS Software:

- **Prediction model type full**
  – A Prediction model type full contains all the information necessary to create, optimize and validate the prediction model. It can be edited and saved. When publishing a prediction model, the OMNIS Software creates a Prediction model type light.
- **Prediction model type light**
  – A Prediction model type light contains only the data for the calculation or reevaluation of the constituent values. In addition, the data preprocessing and wavelength ranges used can be viewed. *Reevaluating the prediction (see chapter 5.8.23.1, page 256)*, *PREDICT – Parameters (see chapter 5.9.4.3, page 447)*
    In the overview list, the last published Prediction model type light is displayed in the **Last published version** column.

NOTICE

If a Prediction model type light is imported into the OMNIS Software for which there is no Prediction model type full in the overview list, it is displayed in the **Type** column as **light**.

See also

Data preprocessing – Area (chapter 5.11.1.11, page 890)

Histogram – Area (chapter 5.11.1.9, page 889)

Influence plot – Area (chapter 5.11.1.16, page 902)

Editing a Prediction model (chapter 5.11.1.5, page 875)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Prediction model – Tab (chapter 5.2.8, page 112)

Prediction model navigator – Functional description (chapter 5.11.1.6, page 883)

Correlation plot – Area (chapter 5.11.1.15, page 898)

Report template – Directory (chapter 5.8.1.4, page 155)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Spectra list – Area (chapter 5.11.1.8, page 886)

Spectra overlay – Area (chapter 5.11.1.10, page 890)

Figures of merit – Definition (chapter 5.11.1.14, page 896)

Wavelength range – Area (chapter 5.11.1.12, page 892)

5.11.1.2 Follow-up of the Prediction model

Reference values of samples that the prediction model is based on can be changed directly in the sample list while editing.

Reprocessing samples

Prerequisite:

- The samples are used in a prediction model.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Opening a sample list

- Identify the samples that the prediction model is based on in **Samples ► Sample lists**.

- Open the sample list.

2 Changing a reference value

- Change the required reference value in the sample data 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, click on in **Results ▶ Calculations** and adjust the required settings.
- Save the sample list by clicking on .

3 Updating a prediction model

- Open the prediction model in question in **Models ▶ Prediction models**.

The message **Prediction model modified** appears. Clicking on **[OK]** updates the prediction model.

4 Checking and re-publishing the prediction model

- Check the data in all the process steps of the prediction model navigator and make any necessary changes. *Editing a Prediction model (see chapter 5.11.1.5, page 875)*
- Check the grayed out data in **Prediction model ▶ Validate prediction model** and recalculate the prediction model by clicking on **[Calculate]**.
- Save the prediction model by clicking on and then re-publish it, if necessary. *Publishing a prediction model (see chapter 5.11.1.17, page 903)*

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Sample list – Tab (chapter 5.2.3, page 100)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Publishing a prediction model (chapter 5.11.1.17, page 903)

Follow-up of the Prediction model (chapter 5.11.1.2, page 867)
Follow-up of the Prediction model (chapter 5.11.1.2, page 867)

Preparing the Prediction model (chapter 5.11.1.3, page 869)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

Exporting a prediction model (chapter 5.11.1.18, page 904)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Audit trail – Directory (chapter 5.12.1, page 917)

5.11.1.3 Preparing the Prediction model

These instructions describe the steps to prepare a data set for the creation of a prediction model.

NOTICE

A method with a minimum of one **MEAS SPEC** command is needed, to obtain an eligible data set. *Creating and editing a method (see chapter 5.9.2.3, page 284)*

These instructions describe 3 options how reference values can be entered before or during a measurement of the samples.

- *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: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Creating a sample profile

- Create a new sample profile under **Samples ▶ Sample profiles**. *Creating and editing a sample profile (see chapter 5.8.4.1, page 176)*
- 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 prediction models that can be created with the sample.

2 Defining the reference parameters

- 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 **Type of input field** field.
- Activate the **Editable field** check box so that the reference values can be entered in **Step 3**.

- In the **Operating procedures / subsamples** area, select the required operating procedure and enter the required number of subsamples.
- Save the sample profile by clicking on .

3 Editing a sample list

- In **Samples ▶ Sample lists**, create a new sample list or open an existing sample list. *Creating and deleting a sample list (see chapter 5.8.1.1, page 142)*
- Select the sample profile and add the required number of samples to the sample list by clicking on .
- Replace the default values with the real values of the available reference samples in the input fields of the reference parameters.
- Save the sample list by clicking on .

Entering reference values with the REQUEST command

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Creating a sample profile

- Create a new sample profile under **Samples ▶ Sample profiles**. *Creating and editing a sample profile (see chapter 5.8.4.1, page 176)*
- 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 prediction models that can be created with the sample.

2 Defining the reference parameters

- 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 **Type of input field** field.
- In the **Operating procedures / subsamples** area, select the required operating procedure and enter the required number of subsamples.
- Save the sample profile by clicking on .

3 Entering and parameterizing the REQUEST command

- Create a new method or open an existing method. *Creating and editing a method (see chapter 5.9.2.3, page 284)*
- Insert a **REQUEST** command in the method. Parameterize the command in such a way that it writes to the sample data. *REQUEST – Parameters (see chapter 5.9.4.16.12, page 609)*

The **REQUEST** command can be executed in the same operating procedure that is to be used for acquiring the spectrum. However, this is not mandatory. What is important is that the **REQUEST** command was executed before the spectrum was acquired or the determination run was completed.

NOTICE

Additional information:

Creating and editing an operating procedure (see chapter 5.9.1.3, page 265)

Creating and editing a sample profile (see chapter 5.8.4.1, page 176)

Creating and deleting a sample list (see chapter 5.8.1.1, page 142)

Starting a determination (see chapter 5.8.6.6, page 207)

4 Entering the reference values

- The reference values can be entered into the corresponding fields during the determination of the sample in **Samples ▶ Sample lists ▶ Curves and data ▶ Live data**.

Entering the reference values from the primary processes with the CALC command

Prerequisite:

- The **MEAS SPEC** command is used in addition to another procedure, e.g. a titration. Ideally, the procedures are split over more than one subsample.

- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Entering and parameterizing the CALC command

- Create a new method or open an existing method. *Creating and editing a method (see chapter 5.9.2.3, page 284)*
  Insert a **CALC** command in the method. Parameterize the command in such a way that it writes to the sample data. *CALC – Parameters (see chapter 5.9.4.16.1, page 586)*

NOTICE

Only reference parameters that were previously defined as field in the sample profile can be selected. In order for the input field to be used as a reference parameter for a prediction model, the units of the input field, the result of the **CALC** command and the reference value have to match.

NOTICE

The **CALC** command can be executed in the same operating procedure that is to be used for acquiring the spectrum. However, this is not mandatory. What is important is that the **CALC** command was carried out before the prediction model was created.

During the determination, the values that were determined as reference parameters by the primary procedure are written in the sample data.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

CALC – Parameters (chapter 5.9.4.16.1, page 586)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Publishing a prediction model (chapter 5.11.1.17, page 903)

Importing the Prediction model (chapter 5.11.1.19, page 905)

Sample list – Tab (chapter 5.2.3, page 100)

REQUEST – Parameters (chapter 5.9.4.16.12, page 609)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

5.11.1.4 Creating a Prediction model

Prerequisite:

- The license to create and edit prediction models is available.
- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Creating a new prediction model

- In **Models ▶ Prediction models**, click on .

The **Create prediction model** dialog opens.

2 Entering a name

- Enter the required name in the input field.

> **NOTICE**
>
> The name can be changed at any time in **Prediction model ▶ Properties ▶ General**.

3 Selecting the samples

- Display all the sample lists saved in the database in the table by clicking on **[Sample lists]**.
  or
- Display all the search queries saved in the database in the table by clicking on **[Search queries]**.
- Select at least one entry in the table to use the spectra in the sample list or search query to create the prediction model.

Depending on which sample list or search query is selected, different entries are available in the **Reference parameter/unit** list.

4 Selecting the reference parameter/unit

- Select a reference parameter from the list that is available for the selected sample list or search query.

NOTICE

Reference parameters of samples that the prediction model is based on can be changed directly in the sample list as necessary while editing.

5 Confirming entries

- Create the new prediction model by clicking on **[Create]**.

The spectra of the sample lists or search queries are loaded into the prediction model with the associated reference parameters.

The new prediction model can be edited further.

6 Editing the prediction model

- Go through the individual process steps of the prediction model navigator and adjust the data as desired. Further information on editing prediction models: *Editing a Prediction model (see chapter 5.11.1.5, page 875)*

7 Saving the prediction model

- Save the prediction model by clicking on .

The prediction model is saved. The version and change date of the prediction model are updated automatically in **Properties ▶ General**.

8 Publishing a prediction model

- Publish the prediction model by clicking on . Further information on publishing prediction models: *Publishing a prediction model (see chapter 5.11.1.17, page 903)*

NOTICE

To use the prediction model in determinations and repredictions, the prediction model must be published.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Sample list – Tab (chapter 5.2.3, page 100)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Publishing a prediction model (chapter 5.11.1.17, page 903)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

Exporting a prediction model (chapter 5.11.1.18, page 904)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Audit trail – Directory (chapter 5.12.1, page 917)

5.11.1.5 Editing a Prediction model

A prediction model is edited in 3 steps:

- *Select samples*
- *Parameterize prediction model*
- *Validate prediction model*

Selecting the samples

Prerequisite:

- The license to create and edit prediction models is available.
- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*
- The **Models ► Prediction models** subsection is opened.
- A prediction model is open and at the front. The prediction model navigator is in the process step **Select samples**.

NOTICE

Further information on the prediction model navigator: *Prediction model navigator – Functional description (see chapter 5.11.1.6, page 883)*

1 Splitting the data set

- Split the data set manually or automatically in **Select samples ▶ Spectra list**.

  Split data set automatically:
  - Open the **Automatic splitting of data set** dialog by clicking on .
  - Check the **Detect outliers** check box to automatically assign spectra to the outlier data set.
  - In the **Percentage of validation data set** field, define the desired percentage of spectra in the validation data set compared with spectra in the calibration data set.
  - If necessary, manually reprocess the automatically split data set.

  Split the data set manually:
  - Right-click on a spectrum in the list to open the context menu and assign the spectrum to the **Calibration data set**, **Validation data set** or **Outlier data set**.
  - To select multiple spectra at once, the following options are available:
    Hold down the **[CTRL]** key while clicking spectra with the left mouse button.
    To select an entire section, select the first value with the left mouse button and, while holding the **[SHIFT]** key pressed down, left-click on the last value of the section. Alternatively, move over the desired spectra in the list with the left mouse button pressed down.
    If a spectrum is selected, then clicking on another sample or subsample while holding the **[CTRL]** key and **[SHIFT]** key pressed down will select all spectra that lie in between.
  - To select all spectra in the spectra list, click in the Spectra list and press the **[CTRL]**+**[A]** keys.
  - Proceed in this way until the desired number of samples from the list is assigned.

NOTICE

At least 2 spectra must be assigned to the calibration data set so that the prediction 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, **blue** highlighting indicates that a spectrum is assigned to the calibration data set. Spectra in the validation data set are indicated by **green** highlighting. Spectra in the outlier data set are indicated by **red** highlighting.

In the **Spectra list** area, the assignments are represented by the following icons:

- spectrum is part of the calibration data set
- spectrum is part of the validation data set
- spectrum is part of the outlier data set

2 Adding other spectra (optional)

- Add other spectra to the spectra list by clicking on .
- Display all the sample lists saved in the database in the table by clicking on **[Sample lists]** in the **Select spectra** dialog.
  or
- Display all the search queries saved in the database in the table by clicking on **[Search queries]**.
- Select at least one entry in the table to use the spectra in the sample list or search query to create the prediction model.
- Click on **[Load]** to load spectra from the selected sample list or search query into the spectra list.

NOTICE

If the selected sample list or search query does not contain any matching spectra, an error message will appear.

To remove spectra from the spectra list, select a spectrum in the spectra list and click on .

3 Editing the properties

- Open the properties of the spectra list by clicking on .

- Select the desired reference parameter for the prediction model under **Properties ▶ Reference parameters** in the **Reference parameter/unit** field.
- In the **Decimal places** field, define the desired number of decimal places for the result values of the prediction model and of the **PREDICT** command.
- Select the desired cross-validation method from the list under **Properties ▶ Cross-validation** in the **Cross-validation method** field.
- Define the desired percentage under **Properties ▶ Outlier limits** in the **Significance level** field.

NOTICE

Further information on the properties of the spectra list: *Spectra list – Properties (see chapter 5.11.1.8.1, page 888)*

The selected options and entered values will be applied in a subsequent step when calculating the prediction model.

Parameterizing the prediction model

Prerequisite:

- The **Models ▶ Prediction models** subsection is opened.
- A prediction model is open and at the front.
- All actions in the **Select samples** process step have been executed.

1 Change to the "Parameterize prediction model" process step

- In the calibration model navigator, change to the next process step of editing the prediction model by clicking on **Parameterize prediction model**.

The **Spectra overlay**, **Data preprocessing** and **Wavelength range** areas become visible.

2 Adding data preprocessing

- Add data preprocessing under **Parameterize prediction 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 desired type of data preprocessing and fill in the corresponding fields.

NOTICE

Further information on different data preprocessing methods and their parameters: *Data preprocessing – Area (see chapter 5.11.1.11, page 890)*

The preprocessed spectra are shown immediately in the **Spectra overlay** area.

3 Defining the wavelength range

- Add a wavelength range under **Parameterize prediction model ▶ Wavelength range** 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.
- Set the wavelength range using the **Spectra overlay** range:
  - Click on **[Activate moving]** in the **Spectra overlay** section.
  - Click on the desired wavelength range in the **Start wavelength** column in the **Wavelength range** 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.

NOTICE

The wavelength ranges may not overlap.

NOTICE

A minimum difference of 5 nm between start wavelength and end wavelength must be observed.

When defining the wavelength range using the **Spectra overlay** area, the values in the fields in the **Wavelength range** area are automatically adjusted.

The wavelength ranges are immediately displayed in the **Spectra overlay** area.

4 Calculating the prediction model

- Calculate the prediction model by clicking on **[Calculate]**.

NOTICE

For very large spectra lists, this step may take some time, especially when using the **Leave-One-Out** cross-validation method. During this time the **[Calculate]** button is inactive.

NOTICE

If the **[Calculate]** button is inactive although no calculation is running at the moment, the following causes may be present:

- The prediction model has already been calculated and no changes have been made since then.
- An incorrect entry was made in one of the process steps. In the calibration model navigator, the process step of the affected area is displayed in **red**. The field with the incorrect entry is outlined in red.

The **[Calculate]** button becomes inactive.

The calculated data are displayed under **Validate prediction model** in the **Figures of merit**, **Correlation plot** and **Influence plot** areas.

Validating the prediction model

Prerequisite:

- The **Models ▶ Prediction models** subsection is opened.
- A prediction model is open and at the front.
- All actions in the **Select samples** process step have been executed.
- The prediction model has been calculated.

1 Switching to the "Validate prediction model" process step

- In the calibration model navigator, change to the next process step of editing the prediction model by clicking on **Validate prediction model**.

The **Figures of merit**, **Correlation plot** and **Influence plot** areas become visible.

2 Selecting the required number of latent variables

- Select the required number of latent variables in **Validate prediction model ▶ 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.

NOTICE

The number of latent variables affects the quality of the calculated prediction model.

Further information on figures of merit: *Figures of merit – Definition (see chapter 5.11.1.14, page 896)*

The number of latent variables is indicated by ✓ in the table. If the number of latent variables selected by the user differs from the number suggested by the system, the suggested number is indicated by →.

In the **Correlation plot** area, depending on the number of latent variables, the curve changes as well as the calculated value. This allows the quality of the prediction model to be checked.

3 **Evaluating and revising the prediction model (optional)**

NOTICE

Any change to the assignment of the spectra (including addition and removal of spectra) necessitates a recalculation of the prediction model. More extensive changes should be made in the **Parameterize prediction model** process step.

- In **Validate prediction model ▶ Correlation plot**, right-click on a spectrum in the chart to open the context menu and assign the spectrum to the **Calibration data set**, **Validation data set** or **Outlier data set**.
- To show or hide outliers, right-click in the **Correlation plot** area and select **[Show/hide outliers]** in the context menu.
- In **Validate prediction model ▶ Influence plot**, right-click on a spectrum in the chart to open the context menu and assign the spectrum to the **Calibration data set**, **Validation data set** or **Outlier data set**.
- Recalculate the prediction model by clicking on **[Calculate]**.

The recalculated data is displayed in the **Validate prediction model** process step. The selection of the number of latent variables may have to be performed again (see step 2).

4 **Recalculating the prediction model (optional)**

- If changes have been made to the assignment of spectra to the various data sets, or spectra have been added to or removed from the spectra list, recalculate the prediction model by clicking on **[Calculate]**.

5 **Saving the prediction model**

- Save the prediction model by clicking on .

The prediction model is saved. The version and change date of the prediction model are updated automatically in **Properties ▶ General**.

> **NOTICE**
>
> To use the prediction model in determinations and repredictions, the prediction model must be calculated and published.
>
> Further information on calculating prediction models: *Publishing a prediction model (see chapter 5.11.1.17, page 903)*
>
> Further information on publishing prediction models: *Publishing a prediction model (see chapter 5.11.1.17, page 903)*

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Sample list – Tab (chapter 5.2.3, page 100)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Publishing a prediction model (chapter 5.11.1.17, page 903)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

Exporting a prediction model (chapter 5.11.1.18, page 904)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Audit trail – Directory (chapter 5.12.1, page 917)

5.11.1.6 Prediction model navigator – Functional description

The prediction model navigator is a horizontal navigation bar and is used to help develop the prediction model in the OMNIS Software.

The user can navigate in both directions between the following steps. Depending on the selection, different areas are displayed:

- **Select samples**:
  - Spectra list
  - Histogram
  - Spectra overlay
- **Parameterize prediction model**
  - Spectra overlay
  - Data preprocessing
  - Wavelength range

- **Validate prediction model**
  - Figures of merit
  - Correlation plot
  - Influence plot

NOTICE

The user is alerted to incomplete or missing entries in the individual areas by the process steps of the respective step being displayed in **red**. The process step is displayed in **black** by default, and in **green** when currently selected.

See also

Spectra list – Area (chapter 5.11.1.8, page 886)

Histogram – Area (chapter 5.11.1.9, page 889)

Spectra overlay – Area (chapter 5.11.1.10, page 890)

Data preprocessing – Area (chapter 5.11.1.11, page 890)

Wavelength range – Area (chapter 5.11.1.12, page 892)

Figures of merit – Definition (chapter 5.11.1.14, page 896)

Figures of merit – Area (chapter 5.11.1.13, page 893)

Correlation plot – Area (chapter 5.11.1.15, page 898)

Influence plot – Area (chapter 5.11.1.16, page 902)

5.11.1.7 Prediction model – Properties

Clicking on  under **Models ► Prediction models** opens the **Properties** window. The following information is available in the **General** subsection:

Prediction model	
Name	Name of the prediction model.
Object ID	Identification number of the prediction model.
Version	Version number of the prediction model. A new version is created automatically each time a prediction model is saved.
Created	Time at which the prediction model was created.
Created by	User ID of the user that created the prediction model.

Prediction model	
Saved	Time at which the prediction model was last changed.
Saved by	User ID of the user that changed the prediction model.

Last published version	
Name	Name of the last published version of the prediction model.
Object ID	Identification number of the last published version of the prediction model.
Saved	Time at which the last published version of the prediction model was saved.
Saved by	User ID of the user that last published the prediction model.

Clicking on the icon under **Models ▶ Prediction models ▶ Prediction model** opens the **Properties** window. The following functions are available in the **General** subsection:

Name	Name of the prediction model (can be edited, max. 255 characters).
Object ID	Identification number of the prediction model.
Version	Version number of the prediction model. A new version is created automatically each time a prediction model is saved.
Created	Time at which the prediction model was created.
Created by	User ID of the user that created the prediction model.
Saved	Time at which the prediction model was last changed.
Saved by	User ID of the user that changed the prediction model.

See also

Editing a Prediction model (chapter 5.11.1.5, page 875)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Publishing a prediction model (chapter 5.11.1.17, page 903)

Prediction model – Tab (chapter 5.2.8, page 112)

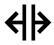
Spectra list – Properties (chapter 5.11.1.8.1, page 888)

Audit trail – Directory (chapter 5.12.1, page 917)

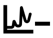
5.11.1.8 Spectra list – Area

In **Models ▶ Prediction models ▶ Select samples ▶ Spectra list**, spectra that are part of the prediction model are tabulated.

The following functions are available:

- 

  Split data set automatically opens the dialog for automatic splitting of the data set.
- 

  Use **Add spectra** to open the dialog for adding spectra to the spectra list.
- 

  Use **Remove spectra** to remove the spectra from the spectra list.
- 

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

The spectra in the spectra list must be split into a calibration data set and a validation data set for external validation of the prediction model:

- Spectra assigned to the **calibration data set** with their constituent values serve as the calculation basis of the prediction model.
- Spectra assigned to the **validation data set** are used with their constituent values to validate the prediction model.
- If spectra or constituent values are erroneous, they can be assigned to the **outlier data set**. This data is not included in the calculation of the prediction model.

NOTICE

Further information on splitting the data set: *Editing a Prediction model (see chapter 5.11.1.5, page 875)*

NOTICE

If values of one of the samples included in the prediction model are changed in the sample list, a message will be displayed in the prediction model. *Follow-up of the Prediction model (see chapter 5.11.1.2, page 867)*

Follow-up of the Prediction model (see chapter 5.11.1.2, page 867)

Preparing the Prediction model (see chapter 5.11.1.3, page 869)

The following information is displayed in the spectra list:

	The spectrum is assigned to the calibration data set.
	The spectrum is assigned to the validation data set.
	The spectrum is assigned to the outlier data set.
	The sample and subsample from which this spectrum and constituent value are obtained are available in the OMNIS Software database.
	The sample and subsample from which this spectrum and constituent value are obtained are not available in the OMNIS Software database. The spectrum and the constituent value are still available in the prediction model.
Sample name	Name of the sample whose spectrum was recorded.
Subsample name	Name of the subsample whose spectrum was recorded.
Command name	Name of the command used to record the spectrum.
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 data set	Display of the number of spectra that is assigned to a calibration data set.
Validation data set	Display of the number of spectra that is assigned to a validation data set.
Outlier data set	Display of the number of spectra that is assigned to a outlier data set.

In the context menu, the following functions are displayed in the spectra list:

	Assign the data set to the **Calibration set**.
	Assign the data set to the **Validation set**.

	Assign the data set to the **Outlier data set**.

See also

Prediction model – Tab (chapter 5.2.8, page 112)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Correlation plot – Area (chapter 5.11.1.15, page 898)

Figures of merit – Area (chapter 5.11.1.13, page 893)

5.11.1.8.1 Spectra list – Properties

Open a prediction model in **Models ▶ Prediction models**. Clicking in the **Spectra list** opens the **Properties** window. In the 3 subsections **Reference parameters**, **Cross-validation** and **Outlier limits**, the following functions and information are available:

Reference parameters

Reference parameter/unit	Select the desired reference parameter with the corresponding unit. Reference parameters can be selected which are available as numeric sample data.
Decimal places	Enter the number of decimal places that are to be displayed for all the calculated and corrected results.

Cross-validation

Cross-validation method	Selecting the desired cross-validation method: ▪ **Leave-One-Out** (default value): The prediction model is validated with Leave-One-Out. A spectrum is obtained from the spectrum dataset. A model is created on the basis of this reduced data set 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. ***Note***: For small spectra lists, the **Leave-One-Out** procedure is recommended. If it is applied to spectra lists with more than 70 spectra, then a warning message will appear. The validation may take a very long time when this procedure is applied. ▪ **K-fold**: The data set is split among random blocks of equal size. Each spectrum is assigned to *one of k*-blocks. Then it is predicted with a model from the other k-1 blocks. If **K-fold** is selected, the following specific parameter appears: – Number of blocks ***Note***: For very large spectra lists, the **K-fold** procedure is recommended.

Number of blocks	Enter the number of blocks in the calibration data set into which the data sets are split. The number of blocks must be smaller than the number of spectra in a calibration data set.
	Outlier limits
Significance level	Enter the desired significance level. 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. Additional information on **Influence plot**: *Influence plot – Area (see chapter 5.11.1.16, page 902)*

See also

Prediction model – Definition (chapter 5.11.1.1, page 866)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Spectra list – Area (chapter 5.11.1.8, page 886)

Influence plot – Area (chapter 5.11.1.16, page 902)

5.11.1.9 Histogram – Area

The distribution of the spectra with respect to a certain constituent value is shown in **Models ▶ Prediction 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 constituent values in **Histogram**. The bin height corresponds to the number of constituent values within the respective interval.

NOTICE

Further information on editing a prediction model: *Editing a Prediction model (see chapter 5.11.1.5, page 875)*

As soon as the **Automatic splitting of data set** function has been executed or data sets have been split manually, the bins of the histogram are displayed in color according to the assignment of the data sets:

Blue	Spectra that are assigned to a **calibration data set**.
Green	Spectra that are assigned to the **validation data set**.
Red	Spectra that are assigned to the **outlier data set**.

See also

Editing a Prediction model (chapter 5.11.1.5, page 875)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Prediction model – Tab (chapter 5.2.8, page 112)

Spectra list – Area (chapter 5.11.1.8, page 886)

Spectra overlay – Area (chapter 5.11.1.10, page 890)

5.11.1.10 Spectra overlay – Area

All spectra of the spectra list are shown overlaid in the **Spectra overlay** area.

The untreated spectra are displayed in **Models ▶ Prediction models ▶ Select samples**. Once a spectrum is selected in the **Spectra list** area, it is highlighted in the **Spectra overlay** area.

Defined wavelength ranges are displayed in the **Spectra overlay** area under **Models ▶ Prediction models ▶ Parameterize prediction model**. 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.

NOTICE

Further information on defining wavelength ranges: *Editing a Prediction model (see chapter 5.11.1.5, page 875)*

See also

Data preprocessing – Area (chapter 5.11.1.11, page 890)

Wavelength range – Area (chapter 5.11.1.12, page 892)

Editing a Prediction model (chapter 5.11.1.5, page 875)

Prediction model navigator – Functional description (chapter 5.11.1.6, page 883)

5.11.1.11 Data preprocessing – Area

In the **Data preprocessing** area, data preprocessings are defined.

- In **Models ▶ Prediction models ▶ Parameterize prediction model ▶ Data preprocessing**, data preprocessings for an open prediction model are defined. The data preprocessings are used for the calculation of the prediction model as well as for the **PREDICT** command that refers to the prediction model. *PREDICT – Parameters (see chapter 5.9.4.3, page 447)*

- In **Processes ▶ Methods ▶ EVAL BASE STATISTICS ▶ Properties ▶ Parameters**, data preprocessings for a **EVAL BASE STATISTICS** command are defined. *EVAL BASE STATISTICS – Parameters (see chapter 5.9.4.11, page 465)*

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 they can be removed with **[Remove data preprocessing]** in the context menu.

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, 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, the following specific parameters appear:	
Derivative order	Entry 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, the following specific parameters appear:	
Derivative order	Entry 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, 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 5.9.4.11, page 465)

Editing a Prediction model (chapter 5.11.1.5, page 875)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Prediction model – Tab (chapter 5.2.8, page 112)

Prediction model – Subsection (chapter 5.11.1, page 864)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

Spectra overlay – Area (chapter 5.11.1.10, page 890)

Wavelength range – Area (chapter 5.11.1.12, page 892)

5.11.1.12 Wavelength range – Area

In the **Wavelength range** area, wavelength ranges are defined.

- In **Models ▶ Prediction models ▶ Parameterize prediction model ▶ Wavelength range**, wavelength ranges for an open prediction model are defined.
- In **Processes ▶ Methods ▶ EVAL BASE STATISTICS ▶ Properties ▶ Parameters**, wavelength ranges for a **EVAL BASE STATISTICS** command are defined. *EVAL BASE STATISTICS – Parameters (see chapter 5.9.4.11, page 465)*

Determining wavelength ranges

Clicking on adds wavelength ranges individually and clicking on removes them again. Up to 10 wavelength ranges can be defined.

NOTICE

In **Models ▶ Prediction models ▶ Parameterize prediction model**, wavelength ranges can also be determined with the **Spectra overlay** area.

Additional information on editing the prediction model: *Editing a Prediction model (see chapter 5.11.1.5, page 875)*

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 5.11.1.11, page 890)

Spectra overlay – Area (chapter 5.11.1.10, page 890)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Prediction model – Tab (chapter 5.2.8, page 112)

EVAL BASE STATISTICS – Parameters (chapter 5.9.4.11, page 465)

5.11.1.13 Figures of merit – Area

The figures of merit are displayed as a chart and as a table in **Models ▶ Prediction models ▶ Validate prediction model ▶ Figures of merit**. Depending on whether the prediction model was calculated with a validation data set, the **SEC. SECV** or **SEC. SECV. SEP** measured quantities are displayed on the y-axis of the chart.

Display of the figures of merit

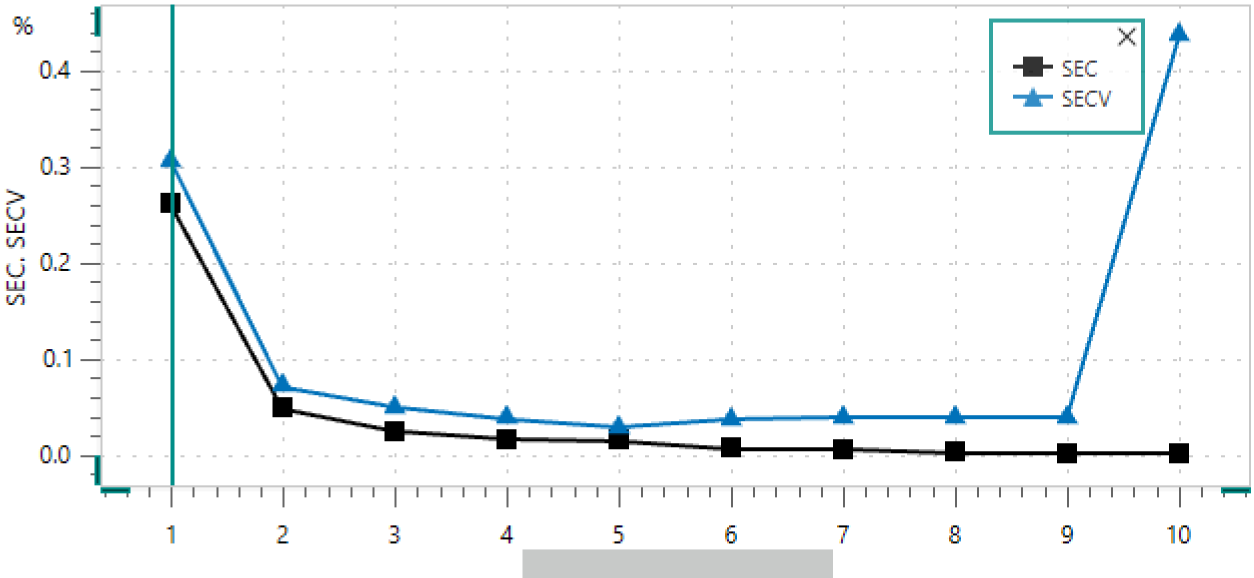
The green vertical line indicates the currently selected number of latent variables. By clicking and moving this line in the chart, the number of latent variables can be edited. The selection is displayed in the table. The selection of a number of latent variables can also be made by double-clicking 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.

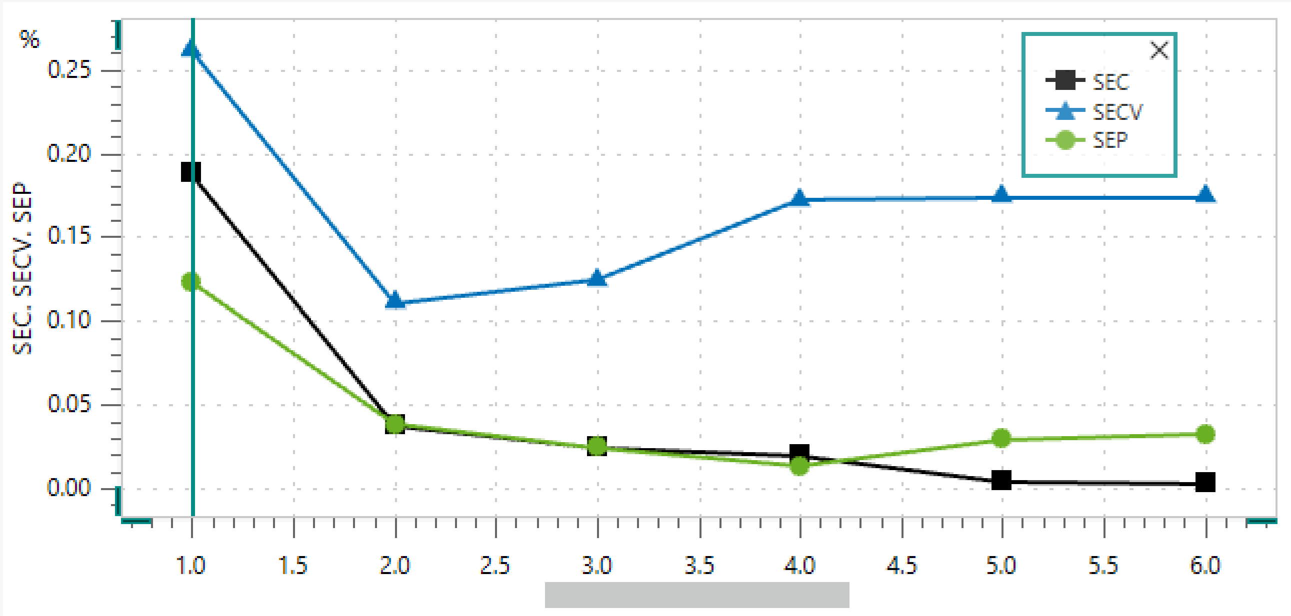
→	Suggested number of latent variables.

If no validation data set has been defined, the following coefficients are displayed in the chart and the table:



Without validation data set	
LV#	Number of latent variables.
SEC	Standard error of calibration.
SECV	Standard error of cross-validation.
R²CV	Correlation coefficient of the cross-validation.

If a validation data set has been defined, the following coefficients are displayed in the chart and the table:



With validation data set	
LV#	Number of latent variables.
SEC	Standard error of calibration.
SECV	Standard error of cross-validation.
SEP	Standard error of prediction.
R²P	Correlation coefficient of prediction.

NOTICE

Further information on the terms **LV#**, **SEC**, **SECV**, **SEP**, **R²P**: *Figures of merit – Definition (see chapter 5.11.1.14, page 896)*

See also

Influence plot – Area (chapter 5.11.1.16, page 902)

Editing a Prediction model (chapter 5.11.1.5, page 875)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Prediction model – Tab (chapter 5.2.8, page 112)

Correlation plot – Area (chapter 5.11.1.15, page 898)

5.11.1.14 Figures of merit – Definition

The figures of merit of the prediction 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 prediction model maps the measuring points of the spectra or associated constituent values with a specific number. The selection of the number of latent variables is crucial for good prediction quality. Too few or too many latent variables lead to inaccurate predictions: If too few latent variables are considered, the variance of the samples will be described incompletely. If too many latent variables are selected, the prediction 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 constituent value and the calculated value based on the calibration data set. A low standard error of calibration indicates that the calibration describes the calibration data set 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 constituent value of *i*, n corresponds to the number of samples from the calibration data set 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 constituent 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 constituent value of *i*, and n corresponds to the number of all samples used to develop the prediction model.

Correlation coefficient of the cross-validation

The correlation coefficient of the cross-validation **R²CV** shows the correlation of the constituent value and the calculated value. The correlation coefficient is determined by cross-validating all samples used to develop the prediction model:

$$r_{y,\hat{y}}^2 = \frac{\left(\sum_{i=1}^{n}(y_i - \bar{y}_i)\cdot(\hat{y}_i - \bar{\hat{y}}_i)\right)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2 \cdot \sum_{i=1}^{n}(\hat{y}_i - \bar{\hat{y}}_i)^2}$$

Here *i* corresponds to the sample, y_i corresponds to the constituent value of *i*, $\bar{y}$ corresponds to the mean value of the constituent 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 prediction 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 the prediction **SEP** shows the standard deviation between the constituent value and the calculated value based on the validation data set:

$$\mathrm{SEP} = \sqrt{\frac{\sum_{i=1}^{v}(\hat{\mathrm{v}}_i - \mathrm{v}_i)^2}{v}}$$

Here *i* corresponds to the sample from the validation data set, $\hat{\mathrm{v}}_i$ corresponds to the calculated value of *i*, v_i corresponds to the constituent value of *i* and v corresponds to the number of samples from the validation data set.

Correlation coefficient of the prediction

The correlation coefficient of the prediction **R²P** shows the correlation of the constituent value and the calculated value, based on the validation data set:

$$r_{y,\hat{y}}^2 = \frac{\left(\sum_{i=1}^{v}(y_i - \bar{y}_i)\cdot(\hat{y}_i - \bar{\hat{y}}_i)\right)^2}{\sum_{i=1}^{v}(y_i - \bar{y}_i)^2 \cdot \sum_{i=1}^{v}(\hat{y}_i - \bar{\hat{y}}_i)^2}$$

Here *i* corresponds to the sample, y_i corresponds to the constituent value of *i*, $\bar{y}$ corresponds to the mean value of the constituent 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 data set.

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

Influence plot – Area (chapter 5.11.1.16, page 902)

Editing a Prediction model (chapter 5.11.1.5, page 875)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Prediction model – Tab (chapter 5.2.8, page 112)

Correlation plot – Area (chapter 5.11.1.15, page 898)

5.11.1.15 Correlation plot – Area

The correlation between **Reference value** and **Calculated value** is displayed graphically in the **Correlation plot** area.

- The slope and the y-axis intercept value of the regression line are displayed in **Models ▶ Prediction models ▶ Validate prediction model ▶ Correlation plot**. If a validation data set was used in the creation of the prediction model, the values of the regression line for this data set are also specified: *Correlation plot in the prediction model*
- The correlation between the constituent value from the primary method and the calculated value or calculated value with slope/y-intercept correction is displayed in **Models ▶ Slope/y-intercept corrections ▶ Correlation plot**: *Correlation plot in slope/y-intercept correction*

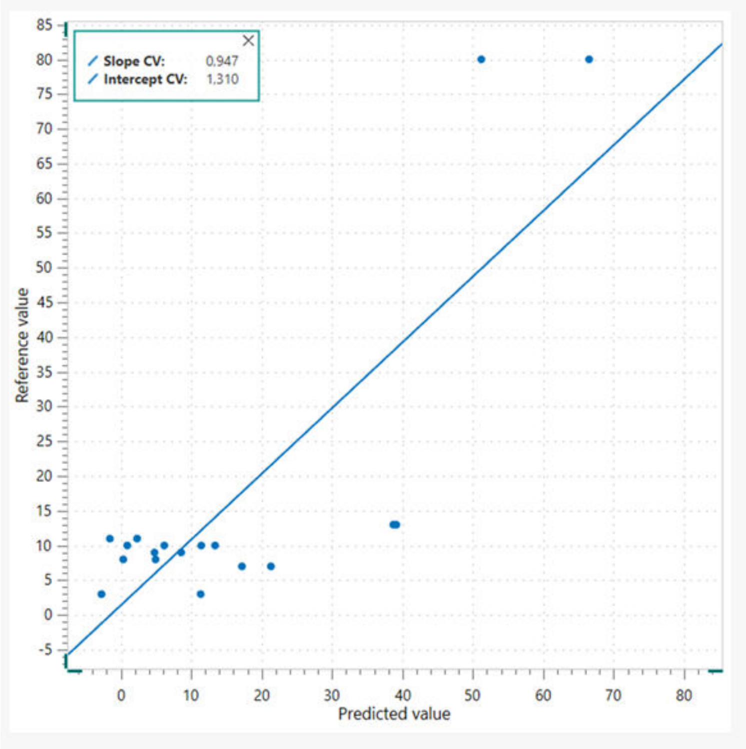
Correlation plot in prediction model

In **Models ▶ Prediction models ▶ Validate prediction model**, the values are displayed as a chart and as a table. Depending on whether the prediction model was calculated with a validation data set, a curve calculated from the validation data set is also displayed in the chart.

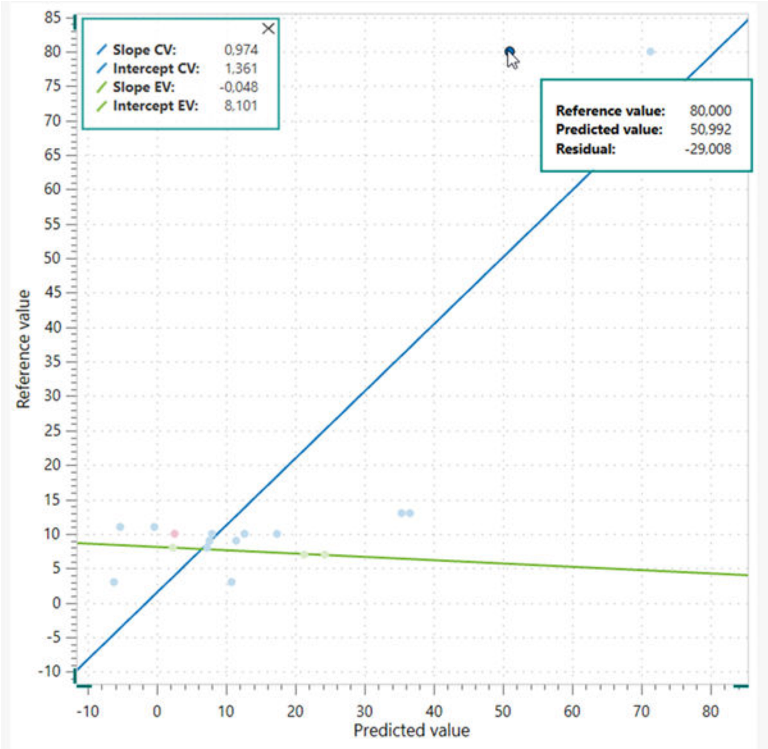
The following values are displayed in the chart:

Without validation data set	
Slope CV	Slope of the regression lines of the values calculated by cross-validation.

Without validation data set	
y-intercept CV	y-intercept of the regression lines of the values calculated by cross-validation.



With validation data set	
Slope CV	Slope of the regression lines based on the calibration data set.
y-intercept CV	y-intercept of the regression lines based on the calibration data set.
Slope EV	Slope of the regression lines based on the validation data set.
y-intercept EV	y-intercept of the regression lines based on the validation data set.



NOTICE

To exclude outliers from the calculation, right-click on a point in the chart to open the context menu and select **[Outlier data set]**. The prediction model must be calculated again afterwards.

Further information on calculating a prediction model: *Editing a Prediction model (see chapter 5.11.1.5, page 875)*

The following values are displayed in the table:

Reference value	Value available for the reference parameter for this sample.
Calculated value	Value that was predicted by using the prediction model on the selected spectrum.
Residual	Difference between calculated value and constituent value.

NOTICE

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 chart in **Models ▶ Slope/y-intercept corrections**. Depending on whether the **Bias correction** or **Slope/y-intercept** option was selected, a different curve is displayed in the chart.

The following values are displayed in the chart, depending on the selection:

Corrected value	Calculated value that was corrected with the bias correction or slope/y-intercept correction.
Calculated value	Value that was predicted by using the prediction model on the spectrum.
Ideal	Ideal line where the regression line has a slope = 1 and the y-intercept = 0.
Slope/y-intercept correction (displayed only when the Slope/y-intercept option is selected)	Curve which is calculated after applying the slope/y-intercept correction.
Bias correction (displayed only when the Bias option is selected)	Curve calculated after applying the bias correction.

The following values are displayed in the details window of the chart:

Reference value	The constituent value of the sample.
Calculated value	Value that was calculated by using the prediction 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	Difference between constituent value and predicted or corrected value.

NOTICE

To exclude outliers from the calculation, right-click on an entry in the **Samples** area to open the context menu and select **[Mark sample as outlier]**.

Further information on creating a slope/y-intercept correction: *Creating and publishing a slope/y-intercept correction (see chapter 5.11.2.4, page 911)*

See also

Editing a Prediction model (chapter 5.11.1.5, page 875)

Histogram – Area (chapter 5.11.1.9, page 889)

Influence plot – Area (chapter 5.11.1.16, page 902)

Figures of merit – Area (chapter 5.11.1.13, page 893)

5.11.1.16 Influence plot – Area

In **Models ▶ Prediction models ▶ Validate prediction model ▶ Influence plot**, notes on possible outliers of the data set after the application of the selected data preprocessing and wavelength selection are displayed. High values for **Hotelling's T²** and **Q residuals** suggest that there might be outliers.

In the **Influence plot** area, the distribution of the data sets as an observational pair of **Hotelling's T²** and **Q residuals** is displayed in the chart. The significance level is also displayed with 2 dashed lines so that spectra can be recognized as outliers more easily.

NOTICE

The significance level is defined in **Select samples ▶ Spectra list ▶ Properties ▶ Outlier limits ▶ Significance level**.

Additional information on the significance level: *Spectra list – Properties (see chapter 5.11.1.8.1, page 888)*

Outliers are highlighted in red. Outliers can be added or changed manually. Spectra or reference values can be assigned manually to the outlier data set, if necessary. To do so, right-click a point in the chart to open the context menu and select **[Outlier data set]**. By holding **[CTRL]** and clicking on additional points, several points can be assigned to the data set at the same time.

See also

Editing a Prediction model (chapter 5.11.1.5, page 875)

Prediction model – Subsection (chapter 5.11.1, page 864)

Prediction model – Tab (chapter 5.2.8, page 112)

Correlation plot – Area (chapter 5.11.1.15, page 898)

Figures of merit – Area (chapter 5.11.1.13, page 893)

Spectra list – Properties (chapter 5.11.1.8.1, page 888)

5.11.1.17 Publishing a prediction model

To use a prediction model for determinations and repredictions, the prediction model must be published. This means that the prediction model can still be developed further without impacting the published version (and the determinations and repredictions carried out with it).

Prerequisite:

- The **Models ▶ Prediction models** subsection is opened. A prediction model is open and at the front.
- The prediction model to be published was calculated and saved.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Opening the dialog

- Open the **Publish prediction model** dialog by clicking on .

2 Updating operating procedures and methods (optional)

- To update methods that use this prediction model, activate the **Update operating procedures/methods** check box.

NOTICE

This option only applies if the existing and already used prediction model was changed and is published again.

Signed methods will not be changed.

3 Publishing a prediction model

- Publish the prediction model by clicking on **[Publish]**.

The last published version of the prediction model is displayed in the overview list and is available for the determination in the parameters of the **PREDICT** command. The prediction model can be used for the reprediction of results.

Additional information on using prediction models in the determination: *PREDICT – Parameters (see chapter 5.9.4.3, page 447)*

Additional information on using prediction models in the reprediction: *Reevaluating the prediction (see chapter 5.8.23.1, page 256)*

NOTICE

If a published prediction model used in a method is deleted, the method cannot be executed anymore.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

Prediction model – Definition (chapter 5.11.1.1, page 866)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Exporting a prediction model (chapter 5.11.1.18, page 904)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

5.11.1.18 Exporting a prediction model

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Exporting a prediction model

- In **Models ▶ Prediction models**, click on .

The **Export prediction model** dialog opens.

2 Selecting the export type

- Select an export type from the selection list in the **Export type** field. Additional information on the export types **Prediction model type full** and **Prediction model type light**: *Prediction model – Definition (see chapter 5.11.1.1, page 866)*

3 Selecting or entering a target folder

- Select a target folder by clicking on 🗁 in the **Target folder** field. Alternatively, enter the target folder path in which the export is to be saved.

4 Defining a file name (optional)

- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

5 Creating an export file

- Click on **[Export]** to create the export file.

The prediction model is exported to the chosen folder.

See also

Editing a Prediction model (chapter 5.11.1.5, page 875)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Publishing a prediction model (chapter 5.11.1.17, page 903)

Importing the Prediction model (chapter 5.11.1.19, page 905)

5.11.1.19 Importing the Prediction model

Prerequisite:

- The OMNIS prediction model file is available.

- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Importing the Prediction model

- Click on to open the **Import prediction model** window in **Models ▶ Prediction models**.

2 Browsing for folder

- Select the folder in which the import file is saved.

3 Selecting the file type

- Select the *.opmo file type at the bottom right of the window.
- Select the import file or enter the name of the import file in the **File name** field.

4 Confirming and importing the selection

- Click on **[Open]** to confirm the selection.

NOTICE

If the prediction model is already available in the database, it can either be overwritten or created as a new version.

The prediction model is imported into the OMNIS Software.

See also

Importing the Prediction model (chapter 5.11.1.19, page 905)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

5.11.2 Slope/y-intercept correction – 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 prediction models or the results of a **PREDICT** command.

- Use **Import slope/y-intercept correction** to import one or multiple slope/y-intercept corrections.
- Use **Export slope/y-intercept correction** to export the slope/y-intercept correction as a file.
- Use **Create report** to create a report of the selected slope/y-intercept correction.
- The properties of the selected element are displayed in the **Properties** window.
- Use **Delete slope/y-intercept correction** to delete the slope/y-intercept correction.

Overview list

The following information is displayed in the overview list:

Name	Name of the slope/y-intercept correction. The name can only be adapted when creating the slope/y-intercept correction.
Used prediction model	The prediction model with which the slope/y-intercept correction is calculated.
Reference parameter/ unit	Reference parameter and unit of the referenced prediction 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.

NOTICE

As soon as the slope/y-intercept correction hast been published, it can neither be opened nor edited.

See also

Prediction model – Definition (chapter 5.11.1.1, page 866)

Reevaluating the prediction (chapter 5.8.23.1, page 256)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Slope/y-intercept correction – Tab (chapter 5.2.9, page 116)

Preparing the Slope/y-intercept correction (chapter 5.11.2.1, page 908)

5.11.2.1 Preparing the Slope/y-intercept correction

These instructions describe the steps to prepare samples for the creation of a slope/y-intercept correction.

Preparing the sample list

Prerequisite:

- A published prediction model with the corresponding reference parameter and the correct unit is available in the OMNIS Software.
- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Entering and parameterizing commands

- Create a new method or open an existing method. *Creating and editing a method (see chapter 5.9.2.3, page 284)*
- Insert a **MEAS SPEC** command in the method. *MEAS SPEC – Properties (see chapter 5.9.4.12.7, page 502)*
- Add at least one **PREDICT** command to the method and reference the prediction model that is to be corrected. *PREDICT – Parameters (see chapter 5.9.4.3, page 447)*
- Save the method by clicking on .

NOTICE

If several reference parameters are to be corrected, more than one **PREDICT** command can be added to the method.

2 Entering the reference parameters

- Write the reference parameters manually with the **REQUEST** command or with the **CALC** command to the sample data. *Follow-up of the Prediction model (see chapter 5.11.1.2, page 867)* *Follow-up of the Prediction model (see chapter 5.11.1.2, page 867)*

  Preparing the Prediction model (see chapter 5.11.1.3, page 869)

NOTICE

The unit and the name of the reference parameters of the prediction model must match the information defined in the fields in the sample profile.

Further information on creating a sample profile: *Creating and editing a sample profile (see chapter 5.8.4.1, page 176)*

See also

Audit trail – Directory (chapter 5.12.1, page 917)

User rights – Directory (chapter 4.6.7.3, page 62)

CALC – Parameters (chapter 5.9.4.16.1, page 586)

Follow-up of the Prediction model (chapter 5.11.1.2, page 867)
Follow-up of the Prediction model (chapter 5.11.1.2, page 867)

Preparing the Prediction model (chapter 5.11.1.3, page 869)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

Sample list – Tab (chapter 5.2.3, page 100)

REQUEST – Parameters (chapter 5.9.4.16.12, page 609)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Slope/y-intercept correction – Definition (chapter 5.11.2.7, page 915)

5.11.2.2 Importing the Slope/y-intercept correction

Prerequisite:

- The OMNIS slope/y-intercept correction file is available.

- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Importing the Slope/y-intercept correction

- In **Models ▶ Slope/y-intercept corrections**, click on .

The **Import slope/y-intercept correction** window opens.

2 Browsing for folder

- Select the folder in which the import file is saved.

3 Selecting the file type

- Select the *.osic file type at the bottom right of the window.
- Select the import file or enter the name of the import file in the **File name** field.

4 Confirming and importing the selection

- Click on **[Open]** to confirm the selection.

The slope/y-intercept correction is imported into the OMNIS Software.

See also

Exporting the Slope/y-intercept correction (chapter 5.11.2.3, page 910)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

5.11.2.3 Exporting the Slope/y-intercept correction

Prerequisite:

- The user has the necessary rights. Further information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Exporting the Slope/y-intercept correction

- In **Models ▶ Slope/y-intercept corrections**, click on .

The **Export slope/y-intercept correction** window opens.

2 Selecting a target folder

- Select the target folder to which the export file is saved.

3 Defining a file name (optional)

- Enter the name under which the file is to be saved in the **File name** field.

> **NOTICE**
>
> The following special characters and character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9.

4 Creating an export file

- Click on **[Save]** to create the export file.

The slope/y-intercept correction is exported to the desired folder.

See also

Importing the Slope/y-intercept correction (chapter 5.11.2.2, page 909)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

5.11.2.4 Creating and publishing a slope/y-intercept correction

Prerequisite:

- The user has the necessary rights. Additional information on user rights: *User rights – Directory (see chapter 4.6.7.3, page 62)*

1 Creating a new slope/y-intercept correction

- In **Models ▶ Slope/y-intercept corrections**, click on .

The **Create slope/y-intercept correction** dialog opens.

2 Entering a name

- Enter the required name in the input field.

> **NOTICE**
>
> The name can be changed in **Slope/y-intercept correction ▶ Properties ▶ General**. After publishing, the name cannot be changed anymore.

3 **Selecting the samples**

- Display all the sample lists saved in the database in the table by clicking on **[Sample lists]**.
  or
- Display all the search queries saved in the database in the table by clicking on **[Search queries]**.
- Select at least one entry in the table to use the samples in the sample list or search query to create the slope/y-intercept correction.

Depending on which sample list or search query is selected, different entries are available in the **Prediction models** list.

4 **Selecting the prediction model**

- Select a prediction model from the list that is available for the selected sample list or search query.

5 **Confirming entries**

- Create the new slope/y-intercept correction by clicking on **[Create]**.

The samples from the sample list or search query as well as the reference value and the calculated value of the prediction model are applied for the calculation of the slope/y-intercept correction.

The new slope/y-intercept correction can be edited further.

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**

- Right-click on individual samples in the **Samples** subsection to exclude the sample from the calculation with **[Mark sample as outlier]**.

NOTICE

To not mark the sample as outlier anymore, right-click on the sample again and click on **[Remove marking of sample as outlier]**.

Alternatively, right-click in the correlation plot and select **[Reset view]** in the context menu.

8 Publishing the slope/y-intercept correction

- Click on to open the **Publish slope/y-intercept correction** dialog.
- Publish the slope/y-intercept correction by clicking on **[Publish]**.

The slope/y-intercept correction is published and saved at the same time. The tab is closed and the slope/y-intercept correction is displayed in the overview list.

NOTICE

A published slope/y-intercept correction can neither be opened nor edited retrospectively.

Additional information on the use of slope/y-intercept corrections in determinations and repredictions: *PREDICT – Parameters (see chapter 5.9.4.3, page 447)Reevaluating the prediction (see chapter 5.8.23.1, page 256)*

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Slope/y-intercept correction – Definition (chapter 5.11.2.7, page 915)

PREDICT – Parameters (chapter 5.9.4.3, page 447)

Creating a Prediction model (chapter 5.11.1.4, page 873)

Audit trail – Directory (chapter 5.12.1, page 917)

5.11.2.5 Slope/y-intercept correction – Properties

Clicking on under **Models** ▶ **Slope/y-intercept corrections** opens the **Properties** window. The following information is available in the **General** subsection:

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 ▶ Slope/y-intercept correction** opens the **Properties** window. The following functions are available in the **General** subsection:

Name	Name of the slope/y-intercept correction (can be edited, max. 255 characters).
Prediction model	Name of the prediction model that is to be corrected.
Reference parameter/unit	Reference parameter and unit of the prediction model that is to be corrected.

See also

Audit trail – Directory (chapter 5.12.1, page 917)

Slope/y-intercept correction – Definition (chapter 5.11.2.7, page 915)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Slope/y-intercept correction – Subsection (chapter 5.11.2, page 906)

5.11.2.6 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.

NOTICE

Further information on the values **Slope**, **y-intercept**, **Bias correction** and **Slope/y-intercept correction**: *Slope/y-intercept correction – Definition (see chapter 5.11.2.7, page 915)*

Further information on the value **SEP**: *Figures of merit – Definition (see chapter 5.11.1.14, page 896)*

See also

Correlation plot – Area (chapter 5.11.1.15, page 898)

Slope/y-intercept correction – Definition (chapter 5.11.2.7, page 915)

Slope/y-intercept correction – Subsection (chapter 5.11.2, page 906)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Slope/y-intercept correction – Tab (chapter 5.2.9, page 116)

5.11.2.7 Slope/y-intercept correction – Definition

If a prediction model creates a systematic error during the prediction of samples with a known reference value, a Slope/y-intercept correction can be created for this prediction 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 either be used during the run of the determination for samples that have not 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**.

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

Prediction model – Definition (chapter 5.11.1.1, page 866)

Reevaluating the prediction (chapter 5.8.23.1, page 256)

Creating and publishing a slope/y-intercept correction (chapter 5.11.2.4, page 911)

Slope/y-intercept correction – Tab (chapter 5.2.9, page 116)

Preparing the Slope/y-intercept correction (chapter 5.11.2.1, page 908)

5.12 Audit trail work area – Actions

The following actions can be executed in the **Audit trail** work area:

- Audit trail entries are filtered, exported and archived in **Audit trail**.

NOTICE

The Audit trail work area is only displayed if the following conditions are fulfilled:

- A valid Software license (**Compliance/Regulation Stand-Alone**) is used.
- The audit trail is activated.
- User management is activated.
- The user has the **Show audit trail** right.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Audit trail – Directory (chapter 5.12.1, page 917)

Filtering Audit trail (chapter 5.12.2, page 922)

Audit trail – Status (chapter 5.12.3, page 924)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Setting up OMNIS Software (chapter 4.3, page 17)

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

5.12.1 Audit trail – Directory

NOTICE

Click on to update the list in the audit trail.

Non-unambiguous objects, e.g. functional units that can change, are displayed as N/A.

Audit trail

Level	Classification of the action. *Audit trail – Status (see chapter 5.12.3, page 924)*
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 that is logged into the OMNIS Software or an external client (e.g. an instrument).
User name	Complete name of the user that is logged into the OMNIS Software or an external client (e.g. an 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.
Client	Name of the computer or instrument on which the action was carried out.

Object properties

Additional information is listed in the object properties. The first five 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.

Further 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.
Operating procedure ID	Unambiguous designation of the operating procedure.
Operating procedure name	Name of operating procedure.
Executed action	Action that was carried out by manual control of the functional unit.
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 which logging into the OMNIS Software or an external client has failed.
Build version	Build version of the OMNIS Software.
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.
Tag ID	Unambiguous designation of the memory chip in the label of the bottle cap.
Firmware version	Version number of the firmware.
Host name	Name of the Cubis II balance in the network.
Prediction model	Name of the prediction model.
Prediction model ID	Unambiguous designation of the prediction model.
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.
Method ID	Unambiguous designation of the method.
Method name	Name of the method.
Package version	Firmware version that is installed on the balance.
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.
Rack code	Rack code of the imported Sample processor rack.

Sensor type	Type of the sensor.
Serial number	Serial number of the product.
Key	Manual control (press of a button) 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 method.

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 saving.

See also

Audit trail work area – Actions (chapter 5.12, page 917)

Filtering Audit trail (chapter 5.12.2, page 922)

Exporting the audit trail (chapter 5.12.4, page 925)

Archiving the audit trail (chapter 5.12.5, page 928)

Audit trail – Status (chapter 5.12.3, page 924)

User rights – Directory (chapter 4.6.7.3, page 62)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Setting up OMNIS Software (chapter 4.3, page 17)

Sorting the overview list (chapter 5.2.10, page 117)

5.12.2 Filtering Audit trail

1 Open the audit trail

- Open the **Audit trail** work area.

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 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.
- **One of the filter criteria must be met**
  - Search results matching at least one filter criterion will be displayed in the list.

4 Add or select filter criterion

- Add additional filter criteria by clicking on .
- Select a filter criterion from the selection list.

NOTICE

Any number of filter criteria can be added to refine the search.

5 Limiting the filter criterion

NOTICE

A filter criterion can be combined with a search operator and a search term.

Depending on the filter criterion, a variety of search operators is available to choose from.

Select a search operator from the selection list and if applicable, also enter a search term, number of days, values, or a date.

- **Contains**
  - The search results contain the entered object.
- **Equals**
  - The search results exactly match the entered object.
- **Does not equal**
  - Only search results that do not match the entered object are displayed in the list.

6 Filtering

- Apply the selected filter criteria by clicking on **[Filter]**.

The results are displayed in the list according to the filter criteria.

7 Resetting filters

- 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.

8 Removing filter criterion

- Remove the filter criterion by clicking on ✕.

NOTICE

If a filter criterion is deleted, then the filter needs to be applied again to see the corresponding entries.

9 Close filters

- Click on ▼ or ↑ to close the filter.

NOTICE

The filter criteria remain active, even after closing the filter.

The area for selecting configurable filter criteria is closed.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Audit trail work area – Actions (chapter 5.12, page 917)

Audit trail – Directory (chapter 5.12.1, page 917)

Sorting the overview list (chapter 5.2.10, page 117)

5.12.3 Audit trail – Status

NOTICE

In the audit trail, you can filter according to a specific level*Filtering Audit trail (see chapter 5.12.2, page 922)*.

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, when exporting the audit trail, when a user logs into the OMNIS Software, when authenticating signatures and when connecting hardware.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Audit trail work area – Actions (chapter 5.12, page 917)

Filtering Audit trail (chapter 5.12.2, page 922)

OMNIS Software – Overview of functions (chapter 5.3, page 119)

Setting up OMNIS Software (chapter 4.3, page 17)

Sorting the overview list (chapter 5.2.10, page 117)

5.12.4 Exporting the audit trail

Prerequisite:

- A valid Software license (**Compliance/Regulation Stand-Alone**) is used.
- User management is activated.
- Audit trail is activated.
- The user has the **Export audit trail** right.
- The **Audit trail** subsection 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.

NOTICE

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: *Filtering Audit trail (see chapter 5.12.2, page 922)*

2 Exporting the audit trail

- Click on to open the window to enter the file name and the target folder.

A new windows opens.

3 Entering the file name

- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

4 Selecting or entering a target folder

- Select the target folder or enter the absolute path in the address bar that the exported file is to be saved in.

5 Creating an export file

- Click on **[Save]**, to create the export file.

The audit trail entries are exported to the chosen folder and an audit trail entry for the steps of the process is created.

NOTICE

This may take several minutes.

The exported file has the valid timestamp of the time at which the export was started by clicking on .

6 Displaying complete and legible entries in HTML format in Microsoft Excel (optional)

- Open the CSV file in Microsoft Excel.
- Select a cell containing HTML data in the **Value** column and double-click to open it.
- Highlight the entire content of the cell with the left mouse button in the editing toolbar.

- Display the context menu with the right mouse button and click on **[Copy]**.
- Add a new sheet.
- Right-click on a cell and select **[Paste Special]** in the context menu.
- In the context menu, click on **[Paste Special]**.
- Select **Unicode Text** in the dialog window 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.

NOTICE

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.

NOTICE

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

User rights – Directory (chapter 4.6.7.3, page 62)

Audit trail work area – Actions (chapter 5.12, page 917)

Filtering Audit trail (chapter 5.12.2, page 922)

Archiving the audit trail (chapter 5.12.5, page 928)

Exporting operating procedure and method (chapter 5.9.1.6, page 272)

Exporting subsample data (chapter 5.8.1.3, page 151)

Archiving samples (chapter 5.8.3.2, page 172)

5.12.5 Archiving the audit trail

Prerequisite:

- A valid Software license (**Compliance/Regulation Stand-Alone**) is used.
- User management is activated.
- Audit trail is activated.
- The user has the **Archive audit trail** right.
- The **Audit trail** subsection is opened.

1 Archiving the audit trail

- Start archiving by clicking on the archive icon and continue the process by clicking on **[Archive]**.

A new windows opens.

> **NOTICE**
>
> 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 the file name

- Enter the name under which the file is to be saved in the **File name** field.

> **NOTICE**
>
> The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, CON, PRN, AUX, NUL, COM1–COM9, LPT1–LPT9

3 Selecting or entering a target folder

- Select the target folder or enter the absolute path in the address bar that the archived file is to be saved in.

4 Creating an archive file

- Click on **[Save]**, to create the archive file.

All the audit file entries are deleted from the current database and an audit entry for the steps of the process is created. The CSV file is exported to and saved in the target folder.

NOTICE

This may take several minutes.

The archived file has the valid timestamp of the time at which the archiving was started by clicking on **[Save]**.

5 Displaying complete and legible entries in HTML format in Microsoft Excel (optional)

- Open the CSV file in Microsoft Excel.
- 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]**.
- Add a new sheet.
- Right-click on a cell and select **[Paste Special]** in the context menu.
- Select **Unicode Text** in the dialog window 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.

NOTICE

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.

NOTICE

All time indications are converted into the 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.

For the date and time displayed in the file name, the local time on the computer is used.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Audit trail work area – Actions (chapter 5.12, page 917)

Filtering Audit trail (chapter 5.12.2, page 922)

Exporting the audit trail (chapter 5.12.4, page 925)

Archiving samples (chapter 5.8.3.2, page 172)

5.13 Settings work area – Actions

You can execute the following actions in the subsections of the **Settings** work area:

- 

  In **Settings ▶ General settings**, the dialog language can be changed and the emergency stop function can be activated or deactivated. A default printer can also be selected and the notification settings can be set.

- 

  In **Settings ▶ Advanced settings**, the system language can be adapted and the User management (OMNIS) or Active Directory can be activated or deactivated. The functions for conformity can also be activated and deactivated 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 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 current database is displayed in **Settings ▶ Data management**.
  If an external database is used on a dedicated Microsoft SQL Server, the connection settings are displayed. These details can also be found in the **OMNIS Database Administration** program on the **Overview** tab.
  If a local database is used, a backup of the currently used database can be created manually and an automatic database backup can be enabled or disabled. In addition, the remaining storage capacity of the selected database is displayed.

NOTICE

If an external database is used on a dedicated Microsoft SQL Server, the **Backup database** and **Automatic database backup** areas are not available. The backup of the database is carried out by an internal IT administrator.

See also

User management (Active Directory) – Actions (chapter 4.5, page 21)
User management (Active Directory) – Actions (chapter 4.5, page 21)

User management (OMNIS) – Actions (chapter 4.6, page 23)

Activating user management (Active Directory) (chapter 4.6.2, page 25)
Activating user management (Active Directory) (chapter 4.6.2, page 25)

Activating user management (OMNIS) (chapter 4.6.3, page 39)

User management settings – Brief description (chapter 4.6.4, page 43)

Setting up notifications (chapter 5.13.2, page 932)

User rights – Directory (chapter 4.6.7.3, page 62)

OMNIS Database Administration – Actions (chapter 6.1, page 936)

Database – Definition (chapter 4.7, page 70)

Setting up a database (chapter 4.7.1, page 72)

Backing up the database (chapter 6.1.2, page 940)

Setting up a printer (chapter 5.13.1, page 932)

Setting up OMNIS Software (chapter 4.3, page 17)

5.13.1 Setting up a printer

1 Selecting a printer

- Select an available physical network printer or local printer from the selection list in **Settings ▶ General settings ▶ Printing settings ▶ Default printer**.

The selected printer is used to print out reports.

> **NOTICE**
>
> Additional information on the 3 options to create reports: *Creating a report (see chapter 5.8.1.5, page 159)*

> **NOTICE**
>
> The printer selection is updated each time the **General settings** subsection is opened or when the OMNIS Software is restarted.
>
> If the required printer is not in the selection list, 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.

See also

Creating a report (chapter 5.8.1.5, page 159)

Operating procedure – Properties (chapter 5.9.1.2, page 262)

REPORT – Parameters (chapter 5.9.4.16.11, page 607)

Setting up OMNIS Software (chapter 4.3, page 17)

User management settings – Brief description (chapter 4.6.4, page 43)

5.13.2 Setting up notifications

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.

NOTICE

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.

NOTICE

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**.

NOTICE

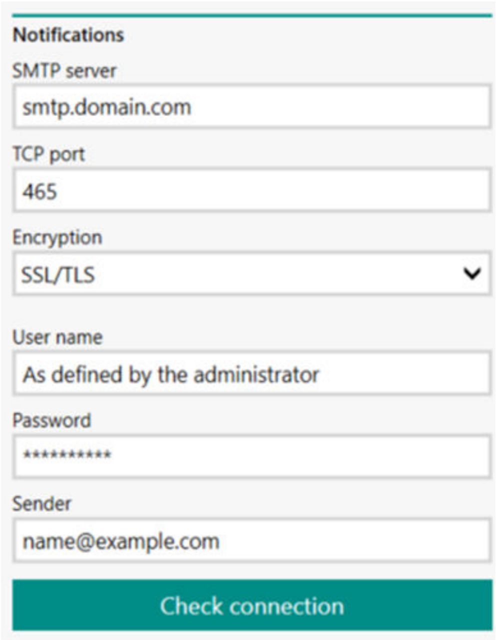
Entering the user name and the password is only necessary, if the SMTP server requires authentication. Otherwise these fields can be left empty.

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.

NOTICE

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.

NOTICE

If the **Audit trail** function in the **FDA 21 CFR Part 11 and EudraLex, Volume 4, Annex 11** option is switched on, then all of the changes made in the Audit trail will be recorded and listed. For more information regarding the recording of entries in the Audit trail, see: *Audit trail – Directory (see chapter 5.12.1, page 917)*

See also

Audit trail work area – Actions (chapter 5.12, page 917)

User rights – Directory (chapter 4.6.7.3, page 62)

User management settings – Brief description (chapter 4.6.4, page 43)

Setting up a printer (chapter 5.13.1, page 932)

Locking conformity (chapter 4.4, page 19)

NOTIFY – Parameters (chapter 5.9.4.16.7, page 599)

Setting up OMNIS Software (chapter 4.3, page 17)

6 Maintenance

6.1 OMNIS Database Administration – Actions

NOTICE

You will need local administrator rights in Windows to execute the **OMNIS Database Administration** program.

Depending on the selected database (local or external database), the following actions can be executed in the tabs:

- 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 ▶ Data management**.
- Under **Back up / Restore**, a backup of the currently used database can be created and backup files can be restored.
  The local database can also be backed up in the OMNIS Software under **Settings ▶ Data management**.
- In **Update / Reset** the database can be updated to a new database version and reset to factory settings (empty database).

NOTICE

If an external database is used on a dedicated Microsoft SQL Server, the **Back up / Restore** tab is not available. Backing up the data and restoring the database is carried out by an administrator.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Updating the database (chapter 6.1.1, page 937)

Database – Definition (chapter 4.7, page 70)

Setting up a database (chapter 4.7.1, page 72)

Backing up the database (chapter 6.1.2, page 940)

Restoring the database (chapter 6.1.3, page 945)

Resetting the database (chapter 6.1.4, page 946)

Settings work area – Actions (chapter 5.13, page 930)

6.1.1 Updating the database

There are 3 options in the OMNIS Software to update the database:

- *(see "Updating the database after installing the OMNIS Software", page 937)*: After having installed the OMNIS Software successfully, the database has to be updated.
- *(see "Updating the database after restoring the database", page 937)*: If the database is out of date, the version of the database must be updated after restoring the database.
- *(see "Message to update the database when starting the OMNIS Software", page 938)*: If the version of the database is out of date, a message is displayed when the OMNIS Software is started.

Updating the database after installing the OMNIS Software

Prerequisite:

- The OMNIS Software is installed.
- The Windows user currently logged on has the local administrator rights.

1 Opening the OMNIS Database Administration program

- Activate the check box in the last dialog window of the installation wizard of the OMNIS Software.
- Exit installation by clicking on **[Finish]**.

The **OMNIS Database Administration** program is opened and a message appears.

2 Updating the database

- Click on **[Update]** in the open message to update the database.

This may take several minutes. The current and the new database now have the same version number.

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.

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.

NOTICE

The version of the database 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, the database cannot be updated anymore. To continue working with the OMNIS Software, the database must be reset or an older database version must be restored.

Message to update the database when starting the OMNIS Software

Prerequisite:

- The Windows user currently logged on has the local administrator rights.

1 Confirm the message

- Confirm the **Database update required** message by clicking on **[Update]**.

Another message appears with the recommendation to back up the database before carrying out the update.

NOTICE

If the database has already been backed up, continue with step 4 *(see "Message to update the database when starting the OMNIS Software", page 938)*.

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.

3 Backing up the database

- Switch to the **Back up / Restore** tab and carry out the backup of the database.

NOTICE

Further information about backing up the database: *Backing up the database (see chapter 6.1.2, page 940)*. 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.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Database – Definition (chapter 4.7, page 70)

Setting up a database (chapter 4.7.1, page 72)

Backing up the database (chapter 6.1.2, page 940)

Restoring the database (chapter 6.1.3, page 945)

Resetting the database (chapter 6.1.4, page 946)

6.1.2 Backing up the database

NOTICE

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.

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. The backup of the database must be carried out by an internal IT administrator.

Back up the database in the OMNIS Software

Prerequisite:

- The local database (Microsoft SQL Server Express) is installed.
- The OMNIS Software is open.
- The user has the **Show data management** right.

1 Selecting the work area

- In the **Settings** work area, open the **Data management** subsection.

2 Entering the file name

- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, 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.

3 Backing up the database

- Back up the database by clicking on **[Back up]**.

The backup file is created in the standard directory **...\Metrohm \OMNIS\MSSQL11.MIAMI\MSSQL\Backup**. This may take several minutes.

Once the backup file has been saved, a message appears.

Backing up the database in the OMNIS Database Administration

Prerequisite:

- The local database (Microsoft SQL Server Express) is installed.
- The OMNIS Software is closed.
- 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 Entering the file name

- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, 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.

4 Backing up the database

- Back up the database by clicking on **[Back up]**.

The backup file is created in the standard directory **...\Metrohm\OMNIS\MSSQL11.MIAMI\MSSQL\Backup**. This may take several minutes.

Once the backup file has been saved, a message appears.

NOTICE

Saving the backup

Database backups are stored on the same drive that the database is installed on. This means that if the computer crashes or the hard drive becomes defective, data could be lost. We recommend copying backed-up files to an external storage medium at regular intervals.

The database backup is created directly by the Microsoft SQL Server. As the Microsoft SQL Server has only limited rights, the backup can only be stored in the default folder.

Example:

The OMNIS Software is installed on the hard disc in the **...\Metrohm\OMNIS\Desktop** directory by default. This means that the database backup is stored in the directory **...\Metrohm\OMNIS\MSSQL11.MIAMI\MSSQL\Backup**.

To automatically store the backup in an external folder, the Windows functionalities or another preferred database backup program must be used.

Automatic database backup from the OMNIS Software

Prerequisite:

- The local database (Microsoft SQL Server Express) is installed.
- The OMNIS Software is open.
- The user has the **Show data management** right.

1 Selecting the work area

- In the **Settings** work area, open the **Data management** subsection.

2 Activating the check box

- 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 Entering the file name

- Enter the name under which the file is to be saved in the **File name** field.

NOTICE

The following special characters or character strings may not be used: >, <, :, ", /, \, |, *, ?, 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.

6 Saving the settings

- Click on **[Apply]** to save the settings.

The backup file is created automatically in the standard directory at the specified time **...\Metrohm\OMNIS\MSSQL11.MIAMI \MSSQL\Backup**. This may take several minutes.

Once the backup file has been saved, a message appears. The date and time of the last successful and the next automatic database backup are displayed.

NOTICE

Saving the backup

Database backups are stored on the same drive that the database is installed on. This means that if the computer crashes or the hard drive becomes defective, data could be lost. We recommend copying backed-up files to an external storage medium at regular intervals. 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 again.

The database backup is created directly by the Microsoft SQL Server. As the Microsoft SQL Server has only limited rights, the backup can only be stored in the default folder.

Example:

The OMNIS Software is installed on the hard disc in the **...\Metrohm \OMNIS\Desktop** directory by default. This means that the database backup is stored in the directory **...\Metrohm\OMNIS \MSSQL11.MIAMI\MSSQL\Backup**.

To automatically store the backup in an external folder, the Windows functionalities or another preferred database backup program must be used.

See also

Audit trail – Directory (chapter 5.12.1, page 917)

User rights – Directory (chapter 4.6.7.3, page 62)

Updating the database (chapter 6.1.1, page 937)

Database – Definition (chapter 4.7, page 70)

Restoring the database (chapter 6.1.3, page 945)

Resetting the database (chapter 6.1.4, page 946)

6.1.3 Restoring the database

NOTICE

If a local database (Microsoft SQL Server Express) is used, the user can restore the database in the OMNIS Database Administration.

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 administrator.

Prerequisite:

- The local database (Microsoft SQL Server Express) is installed.
- The OMNIS Software is closed.
- 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\MSSQL11.MIAMI\MSSQL\Backup**.
- Select the desired backup file.
- Click on **[Open]** to confirm the selection.

The selected database file is displayed in the **OMNIS Database Administration**.

4 Restoring the database

- Restore the database from the backup file by clicking on **[Restore]**.
- Click on **[Continue]** to confirm the subsequent message.

The database is restored from the backup file. This may take several minutes.

Once the database has been restored, a message appears.

> **NOTICE**
>
> The database version might have to be updated after restoring the database. Further information on updating the database: *Updating the database (see chapter 6.1.1, page 937)*

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Updating the database (chapter 6.1.1, page 937)

Database – Definition (chapter 4.7, page 70)

Setting up a database (chapter 4.7.1, page 72)

Backing up the database (chapter 6.1.2, page 940)

Resetting the database (chapter 6.1.4, page 946)

OMNIS Database Administration – Actions (chapter 6.1, page 936)

6.1.4 Resetting the database

> **NOTICE**
>
> If you reset the database, all the data in the database (samples, sub-samples, operating procedures, methods, etc.), device assignments as well as instruments assigned to your settings are lost.
>
> We recommend backing up the existing database before resetting. If an external database is used, the backup of the data is carried out by an administrator.
>
> Further information about backing up the database: *Backing up the database (see chapter 6.1.2, page 940)*.

Prerequisite:

- The OMNIS Software is closed.
- The Windows user currently logged on has the local administrator rights.

1 Starting the OMNIS Database Administration

- 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 **Update / Reset** tab.

3 Resetting the database

- Click on **[Reset]** to reset the database to factory settings.
- Click on **[Continue]** to confirm the subsequent message.

The database will be reset to factory settings (empty database). This may take several minutes.

Once the database has been reset, a message appears.

See also

User rights – Directory (chapter 4.6.7.3, page 62)

Updating the database (chapter 6.1.1, page 937)

Database – Definition (chapter 4.7, page 70)

Setting up a database (chapter 4.7.1, page 72)

Backing up the database (chapter 6.1.2, page 940)

Restoring the database (chapter 6.1.3, page 945)

OMNIS Database Administration – Actions (chapter 6.1, page 936)

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.

Prerequisite:

- The OMNIS Software is installed.
- An Internet connection is available.

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.

NOTICE

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.

NOTICE

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*

NOTICE

Additional information on data storage in the OMNIS Software at: *OMNIS Software – Licensing process*.

See also

OMNIS Software – Faults (chapter 7, page 949)

Collecting OMNIS system information (chapter 9, page 952)

7 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

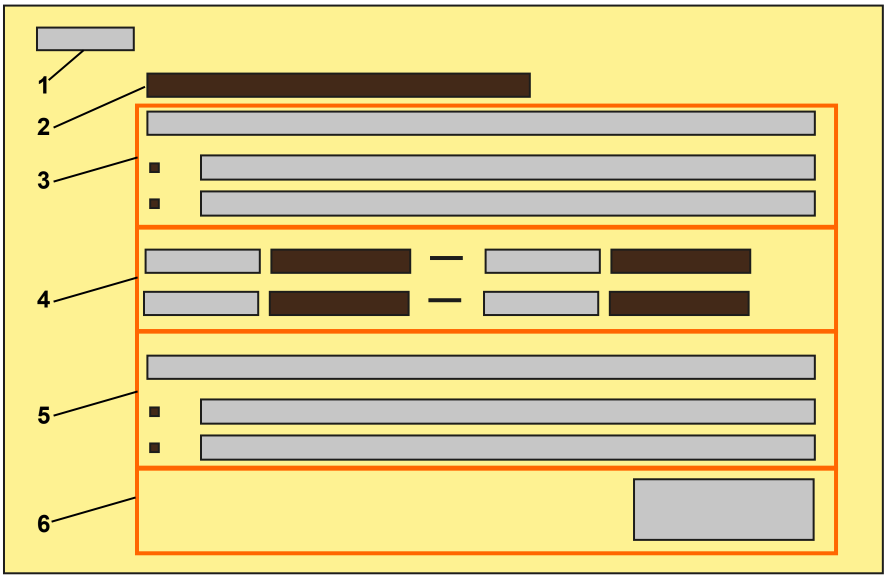
Collecting instrument log files (chapter 10, page 956)

Collecting OMNIS system information (chapter 9, page 952)

Sending OMNIS environment information (chapter 6.2, page 947)

8 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.

NOTICE

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, page 949)

9 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 953)*

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.

NOTICE

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

NOTICE

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

NOTICE

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.

NOTICE

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: *Collecting instrument log files (see chapter 10, page 956)*

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

NOTICE

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

NOTICE

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

NOTICE

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.

NOTICE

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, page 949)

Sending OMNIS environment information (chapter 6.2, page 947)

10 Collecting instrument log files

Prerequisites:

- The user has the **Manage equipment** right.

1 **Opening the 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.

NOTICE

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.

Repeat the steps for all the affected instruments and then start the **OMNIS InfoZipper** program *Collecting OMNIS system information (see chapter 9, page 952)*.

See also

OMNIS Software – Faults (chapter 7, page 949)