MIRA Cal P

Tutorial

8.0105.8004EN / v6 / 2024-09-24

Metrohm

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4.2.XXX

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Table of contents

1 Overview

1.1 Program description

MIRA Cal P software is used together with the Metrohm Instant Raman Analyzers MIRA P and MIRA M-3.

- **MIRA Cal P software**
  Administration (for example users, operating procedures), view results, generate reports, store all data
- **MIRA instruments**
  Analyze samples

Synchronization between MIRA P/MIRA M-3 and MIRA Cal P

With the help of a synchronization workflow, all needed data is synchronized between MIRA Cal P and MIRA P/MIRA M-3.

Synchronizing MIRA P/MIRA M-3 to MIRA Cal P ensures that the instrument is up to date. The current versions of active operating procedures, training sets, libraries and user accounts are transferred to the instrument, while samples and audit trail are saved to the database.

Several instruments can be used, but they ought to be synchronized to the same database in order to achieve a clean data management.

Evaluation

In MIRA Cal P software, 2 evaluation options are available:

- Sample identification
  The measured spectrum of a substance is compared with existing spectra in a library. The best match is reported.
- Sample verification
  This option is used to check if the measured substance corresponds to what was expected.

It is possible to combine both options as well.

Pharma compliant software

- User management
- Electronic signatures of objects
- Audit trail

1.2 Product versions

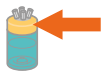
The product is available in the following version:

Table 1 Product versions

Order number	Designation	Version feature
6.0607.1010	MIRA Cal P software	4.2.XXX

1.3 About the documentation

Possible depictions in the documentation:

Depiction	Meaning
*(5-**12**)*	Cross-reference to figure legend (Figure number - ***Element in the figure***)
1	Instruction step
Method	Parameters, menu items, tabs, and dialogs
File ▶ **New**	Menu path
[Continue]	Button or key
	Supplementary information to the descriptive text
	Note In graphics, orange arrows or frames indicate the reference to the descriptive text. The relevant elements may also be colored orange.
	Movement In graphics, blue arrows indicate the movement direction. The elements to be moved may also be colored blue.

1.4 Additional information – Hardware manuals

Refer to following hardware manuals for more information about the instruments:

- MIRA P manual: 8.0924.8001EN
- MIRA M-3 manual: 8.924.8010EN

2 Safety

2.1 Responsibility of the operator

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

- Identify the hazards to the safety and health of its personnel and implement the necessary protective measures and precautions.
- 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 personnel 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.
- Ensure compliance with applicable laws, regulations and standards.

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

- Check the status of the product before use.
- Remedy defects and malfunctions immediately.
- Maintain and clean the product regularly.

2.2 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 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 is present.
- Safety-relevant information is communicated and understood. The personnel can operate the product safely.
- The user documentation has been read and understood. Personnel operate the product according to the instructions in the user documentation.
  CAUTION – Operations, settings or procedures other than those specified in the user documentation may result in hazardous radiation exposure.

2.3 Safety instructions

2.3.1 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.

2.3.2 Danger from radiation

WARNING

Risk of injury by laser radiation

Serious eye injuries by laser radiation.

- Follow the safety measures and instructions.
- Instruments must be used by trained personnel only.
- Instruments of the laser class 3B must be used in protected and labeled rooms only.
- Appropriate protective eyewear according to the technical specifications (see product manual MIRA P, 8.0924.8001) must be used when working with open laser beams (Smart Tips of the laser class 3B).
- Observe the nominal ocular hazard distance (NOHD).
- Follow the provisions of the IEC 60825-1 standard "Safety of laser products" and the regulations for the use of laser systems in your country.

2.4 Design of warning messages

The present documentation uses warning messages as follows.

Structure

1. Severity of the danger (signal word)
2. Type and source of danger
3. Consequences of disregarding the danger
4. Measures for averting the danger

Hazard levels

Signal color and signal word designate the hazard level.

⚠ DANGER

Indicates an immediate danger. It will result in serious injuries or death if not avoided.

⚠ WARNING

Indicates a potential danger. Failure to avoid the danger may result in death or serious injury.

⚠ CAUTION

Indicates a potential danger. If not avoided, it may result in light or minor injuries.

NOTICE

Indicates a potentially damaging situation. If not avoided, the product or something in the surrounding area could be damaged.

2.5 Meaning of warning signs

Warning signs on the product or in the documentation indicate potential dangers or draw attention to certain behaviors in order to avoid accidents or damage.

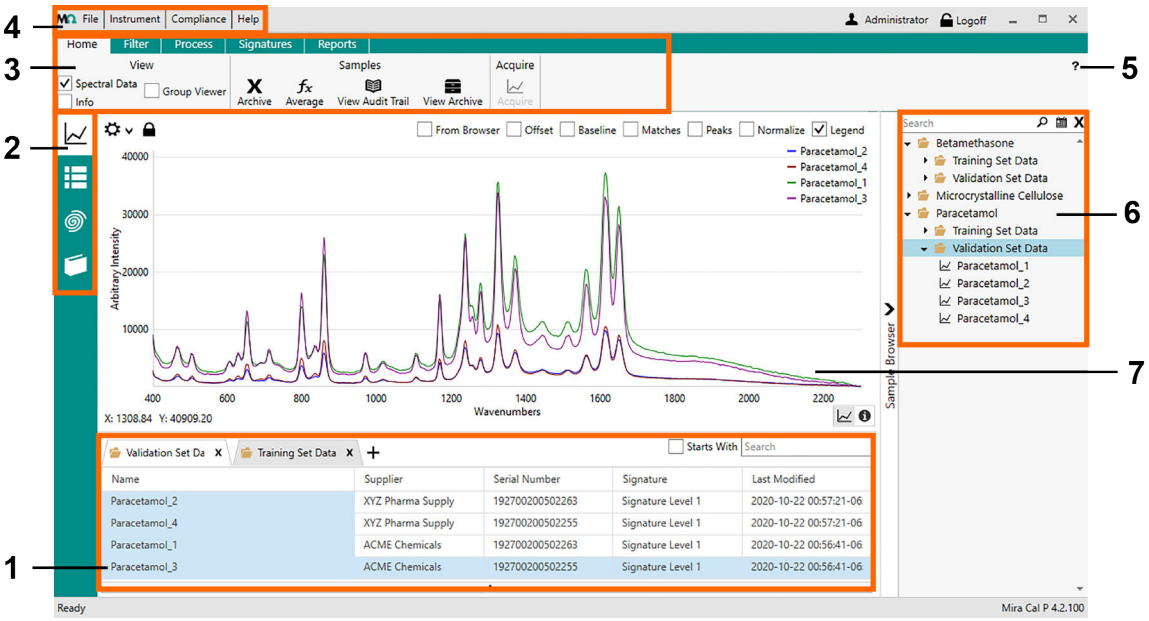
Depending on the application purpose, the operating company attaches additional warning signs to the product. The corresponding instructions of the operator must be followed.

Table 2 Warning signs according to ISO 7010 (examples)

Warning signs / meaning		Warning signs / meaning	
	General warning sign		Warning of hot surface
	Warning of sharp object (cut/ puncture)		Warning of hand injuries (crushing)
	Warning of electrical voltage		Warning of corrosive substances
	Warning of optical radiation		Warning of a laser beam
	Warning of flammable materials		Warning of biological hazard
	Warning of toxic materials		

3 Functional description

3.1 MIRA Cal P – General overview



1 **Sample viewer** with sample lists	**2** **Function tabs** Sample view Library view Training set view Operation procedure view
3 **Ribbon**	**4** **Menu bar**
5 **Contextual help**	**6** **Sample browser**
7 **Spectrum plot and info**	

3.2 MIRA Cal P – Contextual help

Users can find help information directly in the software by clicking ? in the top-right corner of the window in the following locations:

- **Sample** view
- **Library** view
- **Training set** view
- **Compliance configuration**

3.3 Identifying samples with libraries

The measured spectrum of a substance is compared with existing spectra in a library that has been loaded to MIRA P/MIRA M-3.

Libraries can be created by the user or purchased from commercial sources.

Creating a library

Users can create a library in MIRA Cal P, which will then be used for identification of samples. Identification libraries are generated in MIRA Cal P from acquisitions of known substances that the user has access to *(see "Creating and editing libraries", page 24)*.

Purchasing commercial libraries

In addition to user created libraries Metrohm Raman offers different sets of ready-to-use libraries.

Identifying a substance

Libraries are selected for matching when operating procedures are created.

When analyzing a sample, the sample spectrum will be compared to all the spectra in the selected library. The measured sample will be identified as one of the library samples and displayed as **Identification Result**. If there is no match of the sample to a library, **Inconclusive** will be displayed.

3.4 Verifying samples with training sets

This option is used to check if the measured substance corresponds to what was expected.

Typical application for verification analysis: QA/QC applications such as raw material verification before use (**with** prior knowledge/expectation about the samples identity).

Creating a training set

Before sample evaluation, the user must create a training set in MIRA Cal P. This training set is used for verification of samples. A training set consists of different spectra of the substance to be verified. The variance of the measuring process must be reflected in the training set. It is essential that these samples represent the statistical population, that means the variance encountered during analysis must be incorporated in the training set. Failing to select appropriate samples will lead to poor performance. For statistical purposes it is therefore required to measure a minimum of 20 samples *(see "Creating and editing training sets", page 25)*.

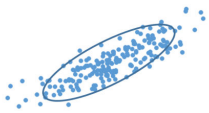
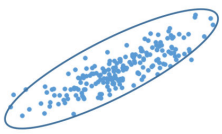
Define confidence interval:

The confidence interval defines the limit between a pass and a fail decision. For example, if a confidence interval of 0.95 is configured, an average of 5% of the measured samples belong to the population outside the defined limit and will be rejected.

A high confidence interval will result in fewer false negatives and increase the probability of false positives.

A low confidence interval will result in fewer false positives (acceptance of inappropriate samples).

Samples are rejected if they lie outside the confidence interval (ellipsis in the following table).

Confidence Interval 0.90	Confidence Interval 0.95	Confidence Interval 0.99
		

When a training set is linked to an operating procedure, the confidence interval can be configured.

Verifying a substance

The measured substance will be evaluated whether it lies within the confidence interval. If so, the identity is confirmed – a pass result will be displayed.

3.5 Operating procedures

MIRA P/MIRA M-3 uses well defined operating procedures from MIRA Cal P.

All parameters that affect the acquisition and evaluation of spectra are defined in operating procedures. This ensures that measurement is done in a tested and reproducible way.

Users build operating procedures in MIRA Cal P and synchronize them to the device before use. Operating procedures can be shared between MIRA P/MIRA-M3 instruments *(see "Creating and editing operating procedures", page 31)*.

3.6 Drop down menus

File	
Open ▶	
Samples	Import samples.
Libraries	Import libraries.
Training Sets	Import training sets.
Operating Procedures	Import operating procedures.
Save As ▶	
Samples	Save samples to selected location.
Libraries	Save libraries to selected location.
Training Sets	Save training sets to selected location.
Operating Procedures	Save operating procedures to selected location.
Advanced ▶	

Database	**Info** Show statistics about the database including: ▪ Number of samples, operating procedures, training sets, libraries ▪ Size of database ▪ Location **Help** Display information on **Database Info** and **Database Reset**. **Back Up** Back up the database. **Restore** Restore the database. **Set Location** Set the location of the database. **Import Licensed Libraries** Import licensed libraries. **Reset** Clear a database without removing users, operating procedures, training sets, libraries, or the compliance configuration. The audit trail remains intact except for the sample-related events. Administrator rights are necessary.
Change Language	Choose the desired language.
Service Portal	Allows access for the regional Metrohm service representative.
Exit	Close MIRA Cal P software.

Instrument	
Connect	Connect MIRA P/MIRA M-3 to MIRA Cal P.
Disconnect	Disconnect MIRA P/MIRA M-3 from MIRA Cal P.
Permissions	View, add, delete or edit instrument permissions.
System Suitability Test Archive	Save and view conducted system suitability tests.
Info	Lists identification information of the instrument and the operating system.
Rename	Change the name of MIRA P/MIRA M-3.
Execute Script	Executes an imported script file.

Calibrate Instrument	Calibrate the instrument. System suitability test can be run immediately following calibration.
System Suitability Test	Conduct a system suitability test. System suitability tests can be run independently of the calibration routine. Follow the prompts.
Updates ►	
Firmware Update	Update firmware.
Update Licensed Libraries	Update licensed libraries.
Upload Language Package	Upload a language package.
Import Certificate Package	Import a certificate package.
Advanced ►	
Upload Encrypted Library	Upload an encrypted library.
Upload Library Access File	Upload a library access file.
Upload S.T. Japan Library	Upload a S.T. Japan library.

Compliance	
Audit Trail	Open the audit trail.
Revert Objects	Opens the archive to revert objects.
Change Password	Change the password.
User Management	Open the user management.
Compliance Configuration	Open the settings.

Help	
About	Displays MIRA Cal P version and copyright.

Create Support File	Create ZIP file for manufacturer to troubleshoot potential issues. This support file will contain information about MIRA Cal P and MIRA P/MIRA M-3 if it is connected.

Connected	Displays when MIRA P/MIRA M-3 is connected to MIRA Cal P.

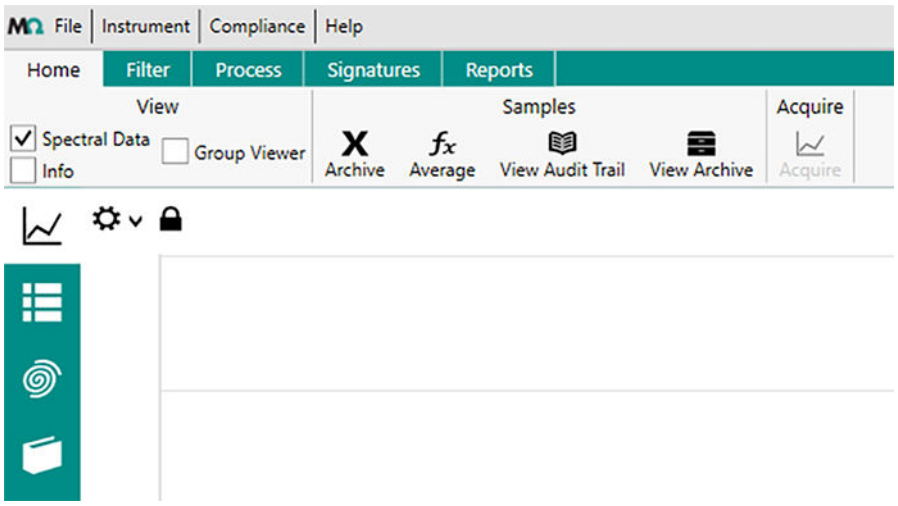
3.7 Function tabs and feature views

The features displayed in the function tabs depend on which view the user has selected from the left side menu. There are the following views.

- **Sample** view
- **Library** view
- **Training Sets** view
- **Operating Procedure** view

Depending on the user role, not all views are visible.

Sample view



Sample **Home ▶** **View**	Select **[Spectral Data]** to view spectral data. Select **[Group Viewer]** to group spectra and view them as a color group. This feature is useful for comparing different vendors, containers, batches etc.

Select **[Info]** to see information regarding metadata, identification results, verification results, reference or signatures.

Under **Info** ▶ **Metadata** copy the GUID to be able to search the audit trail by GUID.

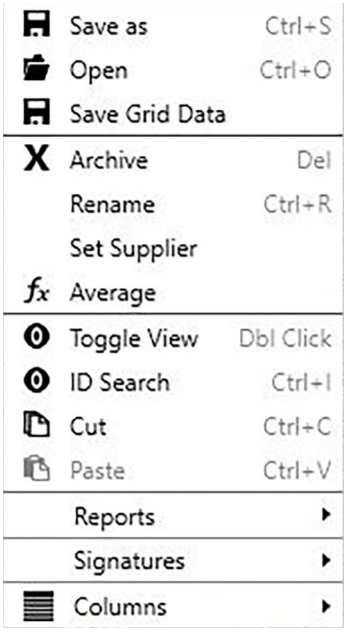
Fill out the metadata **Product ID**, **Lot ID**, **Batch ID**, **Container**, **Supplier** to display them in different colors in the model plots of the training set.

Samples

Click on a sample in the sample list:

- Archive samples
- Average spectra using a fully traceable average function with no loss of information
- View the audit trail
- View the archive

Right click on a selected sample to open a function menu.



Click on **[Set Supplier]** to select multiple samples and set the supplier for all of them at the same time.

Data Set Acquisition

Collect a set number of scans with varying parameters.

Filter

Select parameters to sort samples.

Process

Run Identification, Mixture Matching, or Verification using libraries or training sets that were not defined in the original OP.

Signatures

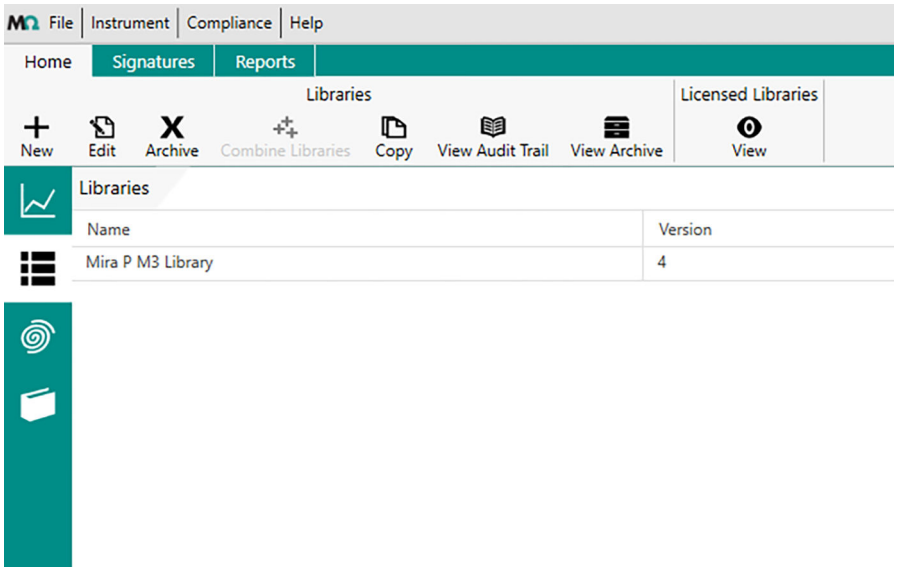
Sign a sample to confirm for example that the sample is approved or reviewed.

Withdraw a signature to confirm for example that the sample is rejected or that sample data is incorrect.

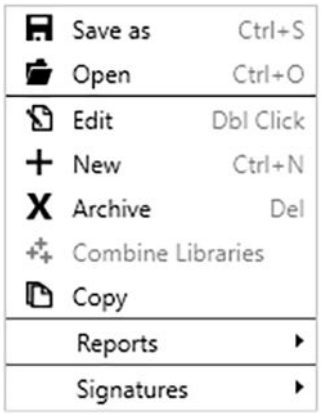
Reports	Generate reports for the selected spectra.

The **[Acquire]** button is active only when MIRA P/MIRA M-3 is connected to MIRA Cal P.

Library view



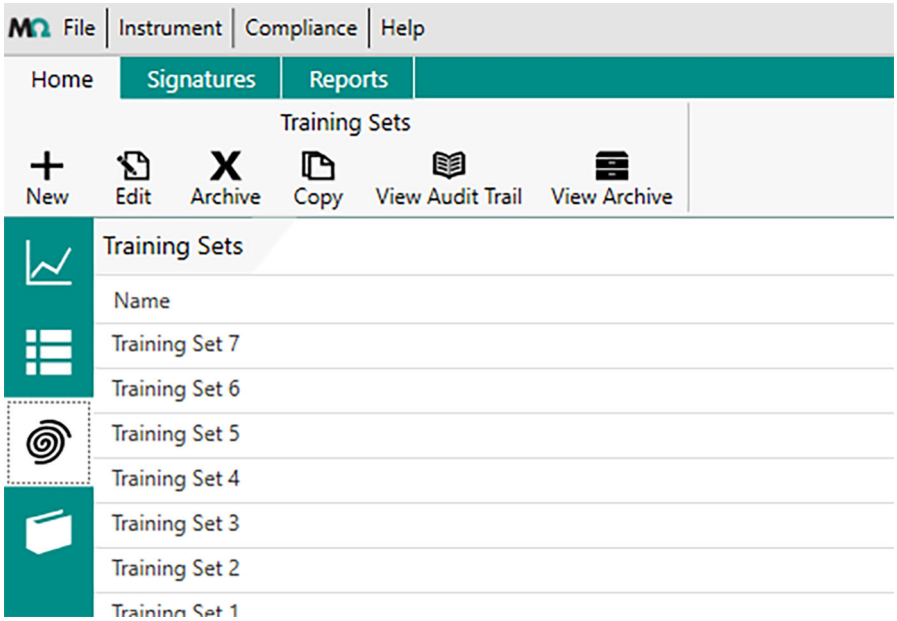
Library	
Home	Click on a library to carry out actions as editing libraries, viewing archived libraries or viewing licensed libraries. Right click on a selected library to open a function menu.



Combine Libraries	Merge multiple libraries. Maintain the original library and add a new one. The function is available after selecting multiple libraries in the **Libraries** window.
Reports	Generate reports for the selected libraries.

Signatures	Sign a library to confirm for example that the library is approved or reviewed. Withdraw a signature to confirm for example that the library is rejected or that sample data is incorrect.

Training sets view

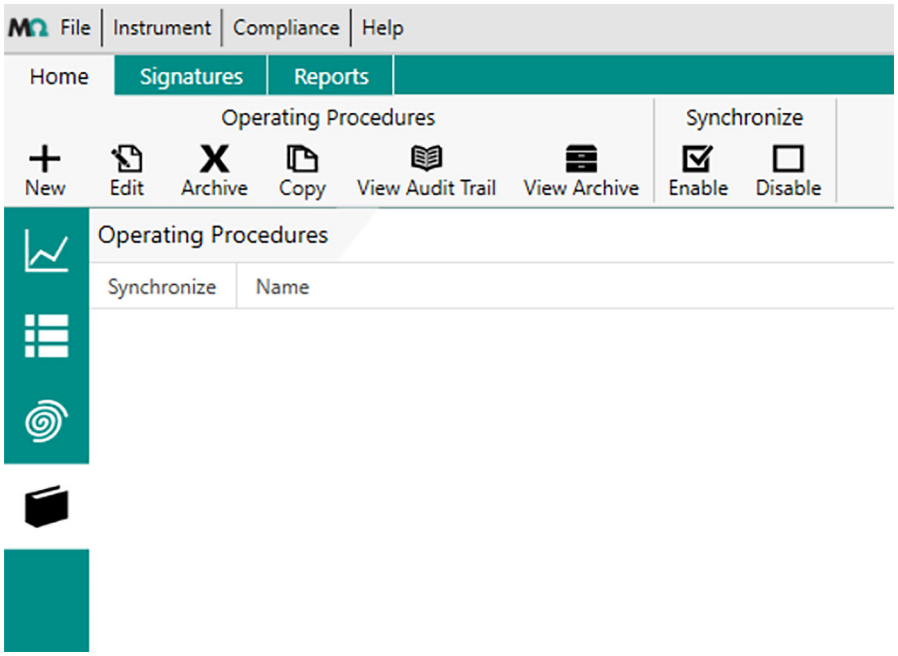


Training Sets	
Home	Click on a training set to carry out actions as editing training sets, archiving training sets or viewing the audit trail. Right click on a selected training set to open a function menu.

Signatures	Sign a training set to confirm for example that the training set is approved or reviewed. Withdraw a signature to confirm for example that the training set is rejected or that sample data is incorrect.

Reports	Generate reports for the selected training sets.

Operating procedure view



Operating Procedures  **Home ▶** **Operating Procedures**	Click on an operating procedure to carry out actions as editing operating procedure, archiving operating procedures or viewing the audit trail. No actions can be taken on the default operating procedure. Right click on a selected operating procedure to open a function menu.

Synchronize	Enable or disable synchronization between MIRA P/MIRA M-3 and MIRA Cal P.
Signatures	Sign an operating procedure to confirm for example that the operating procedure is approved or reviewed. Withdraw a signature to confirm for example that the operating procedure is rejected or that sample data is incorrect.
Reports	Generate reports for the selected operating procedures.

3.8 Sample browser

The Sample browser displays the sample folders and their contents. Selecting and double clicking a folder or sample in the browser will open that object in the sample viewer.

4 Installation

4.1 System requirements

For details on system installation and setting up Windows® permissions, please see the **System Administrator Guide** (0000-9611). Available from your Metrohm Service representative.

Processor	Multicore x86 processor (64-bit)
Operating system	▪ Windows 11 ▪ Windows 10 (64-bit only)
Screen resolution	Resolution 1024 x 768 or higher
RAM	Windows 11: 4 GB minimum Windows 10: 2 GB minimum; 4 GB recommended
Storage capacity	Minimum 100 GB; 500 GB recommended
USB connectors	USB 3.0
Mouse and keyboard	Required, USB, PS/2 style, or wireless
Keyboard	Compatible keyboard using USB / PS/2, or similar connection
System backup	Network or local backup required for data archiving.

Only use the provided Metrohm USB cable (6.021.08010) and do not use third party USB cables. The usage of a powered USB Hub is recommended.

4.2 Installing MIRA Cal P

Make sure, to have administrator rights before installing MIRA Cal P software.

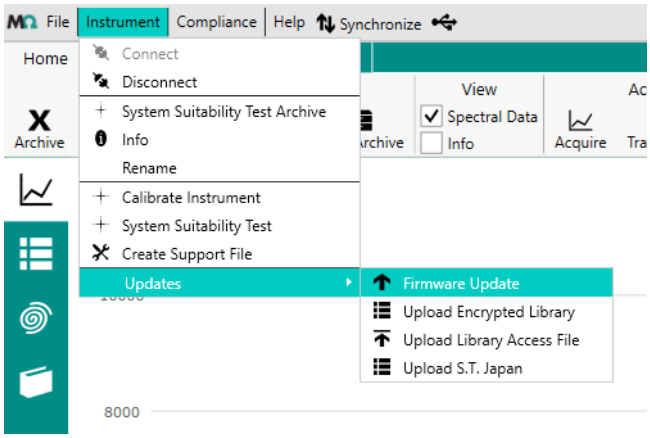
Make sure that the system fulfills the system requirements *(see "System requirements", page 20)*.

1 Double-click on the installer file.

2 Click on **[Install]** and follow the wizard on the screen.

If missing, additional third party software will be installed as well.

4.3 Updating the firmware

1 

Click on **Instrument** ▶ **Updates** ▶ **Firmware Update**.

2 Select the new firmware package (.zip file) on the file system.

3 Click on **[Ok]**, to update the firmware.

Click on **[Cancel]**, to cancel the firmware update.

4 During firmware update, a window is displayed showing the old and the new firmware version.

Click on **[Accept]** to agree to the changes and install the new firmware.

After a firmware update, the instrument must be calibrated again. Information regarding calibration can be found in *"Calibration and system suitability", page 36*.

5 Start-up

5.1 Database conversion

A database conversion takes place if the computer that MIRA Cal P is installed on already has a previous version of MIRA Cal (3.0 or higher). MIRA Cal P uses a new database format.

The first start-up of MIRA Cal P converts the old database to the new format.

MIRA Cal P first prompts the user to make a backup of the old database. Then MIRA Cal P proceeds with the conversion.

The database conversion takes less than 1 hour.

5.2 Starting MIRA Cal P

The initial user name and password are (unless the existing database was converted):
User Name: admin
Password: Change!

1 Double-click on  , to start the program.

After software installation, the MIRA Cal P icon is displayed on the desktop of the computer.

2 Enter your user name and password and click on **[Login]**.

5.3 Connecting to MIRA Cal P

- It is not recommended to use third party USB cables. Only use the provided Metrohm USB cable (article number 6.215.1110).
- The usage of a powered USB Hub is recommended.

Connecting MIRA P/MIRA M-3 via USB

1 Connect MIRA P/MIRA M-3 to the computer by using the USB Mini-B cable.

MIRA P/MIRA M-3 will automatically power on when connected to the host.

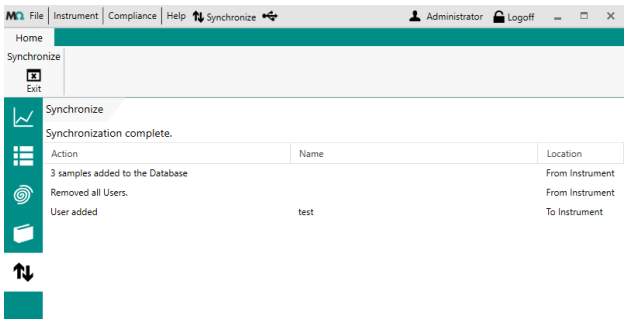
Wait a moment for the instrument to be ready. The login screen displays when MIRA P/MIRA M-3 is ready to be connected to the host.

Connecting MIRA P/MIRA M-3 in MIRA Cal P

1 In the menu tab, select **Instrument** ▶ **Connect**.

The icon  in the menu bar of MIRA Cal P indicates a successful connection.
The screen of the instrument displays **Connected**.

2 If MIRA P/MIRA M-3 is connected to MIRA Cal P, the **[Synchronize]** button appears in the menu bar. Click on **[Synchronize]** to synchronize data between MIRA P/MIRA M-3 and MIRA Cal P.



Synchronization progress appears in an information bar at the bottom of the MIRA Cal P window. When synchronization is complete, the information bar displays **Ready**.

3 To disconnect MIRA P/MIRA M-3 from MIRA Cal P, click on **Instrument** ▶ **Disconnect**.

5.4 Configuration

5.4.1 Creating and editing libraries

Spectra for libraries come from samples that have previously been acquired or imported into the sample database.

Creating a library

1 Go to the **Library** view.

2 Go to the **Home** tab.

3 Click on **[New]**.

4 Add metadata (library information).

After a library is created, its' name cannot be changed.

5 Go to the **Add Samples** tab.

6 Select samples. You can select multiple samples with the key **[CTRL]** and the key **[SHIFT]**.

7 Click on **[Add]**.

8 Click on **[Confusion Matrix]** to see cross-correlation of all library samples.

9 Click on **[Save]** to create the new library.

Editing a library

1 Go to the **Library** view.

2 Select a library and click on **[Edit]**.

3 You can add and delete samples to/from the library.

- To add a sample to the library, go to **Add Samples**. Click on **[Add]**.

- To delete a sample from the library, select a sample. Click on **[Delete]**.

4 Click on **[Save]**.

5 Only libraries that are associated with an active operating procedure will synchronize to the device.

Edited libraries are synchronized in the same manner as newly created libraries.

6 Library sample metadata can be edited in preexisting user libraries.

5.4.2 Creating and editing training sets

Before sample evaluation, the user needs to create a training set in MIRA Cal P. This training set will be used for verification of samples. A training set consists of different spectra of the substance to be verified. The variance of the measuring process must be reflected in the training set.

In MIRA Cal P 4.1.0 and above, the PCA algorithm has been updated to add new features. This update applies to new training sets by default. Existing training sets use the legacy algorithm until the training set is modified in any way.

Table 3 PCA algorithm parameter defaults and options

	Default settings	Options
PCs	2	1 to 5
Pretreatment	Mean Center	Mean Center/None
Distance measure	Combined	Combined / Hotelling T^2 / QResidual
Confidence interval	0.95	0.90 / 0.95 / 0.975 / 0.99
Normalization	SNV Normalize	SNV / Vector / Min-Max
Smooth	Savitzky-Golay: 13 points (27 point window), third-order polynomial	Continuous
Baseline	OFF	ON / OFF
Derivative	ON	ON / OFF
Instrument Variance Compensation (IVC)	ON	ON / OFF

Creating a training set

1 Go to the **Training Sets** view.

2 Go to the **Home** tab.

3 Click on **[New]**.

4 Add metadata (training set information).

After a training set is created, its name cannot be changed.

5 Go to the **Add Samples** tab.

6 Select Samples. You can select multiple samples with the key **[CTRL]** and the key **[SHIFT]**.

A training set must contain at least 20 samples.

7 Click on **[Add]**.

8 Go to the **Validation Set** tab.

9 Click on **[New]** under the **Validation Set** ribbon.

10 Add a name for the validation set. After a validation set is created, its name cannot be changed.

11 Click on the **Sample Browser** tab or the **Recent** tab.

12 Select Samples that should PASS the model. Select multiple samples with **[CTRL]** or **[SHIFT]**.

13 Click on **[Add To Positive]** under the **Validation Set** ribbon.

14 Select Samples that should FAIL the model. Select multiple samples with **[CTRL]** or **[SHIFT]**.

15 Click on **[Add To Negative]** under the **Validation Set** ribbon.

16 Click on **[Save]** under the **Validation Set** ribbon.

17 Go to the **Overview** tab.

18 Click on **[ModelExpert]** in the **Training Set** ribbon.

Finding model settings may take several minutes.

19 Click on **[Save Training Set]** at the bottom of the **ModelExpert** dialog to create the training set.

Editing a training set

1 Go to the **Training Sets** view.

2 Select a training set and click on **[Edit]**.

3 You can add and delete samples to/from the training set.

- To add a sample to the training set, go to **Add Samples**. Click on **[Add]**.
- To delete a sample from the training set, select a sample. Click on **[Delete]**.

4 Click on **[Save]**.

5 Only training sets that are associated with an active operating procedure will synchronize to the device.

Edited training sets are synchronized in the same manner as newly created training sets.

Selecting parameters

1 Go to the **Overview** tab.

2 **ModelExpert** is a tool for determining the best processing methods for a set of data based on a training set and a validation set. There are many types of processing that can be applied to the training set to make the model work for the application such as normalization, centering, derivative etc. **ModelExpert** is the recommended procedure but parameters can be selected manually if desired.

Select **Training Set Model** in the ribbon.

3 Set desired parameters or run **ROC Curves** in the ribbon to see best combinations (validation set required) *(see "Verification tools and recommendations", page 28)*.

5.4.3 Verification tools and recommendations

Verification with MIRA P / MIRA M-3 is based on PCA (Principal Component Analysis) models. PCA works on a Training set, a set of multiple spectra for the same material, and reduces dimensionality by finding similarities between all the spectra in the training set.

Training Sets

A good training set is built for only one material. It is a collection of spectra that represent natural variations that are expected for that material during routine analysis. Variations can come from:

- Suppliers
- Containers
- Devices

The optimal number of tests depends on the variations that the model has to understand. The minimum in the software is 20 but the ideal number is usually about 40 to 80 tests. Training sets are fully-compliant objects in MIRA Cal P. They are version-controlled and can be signed by multiple levels to prevent undesired modifications. The Training set samples are added on the **Add Samples** tab in the **Training Set** editing window.

Validation Sets

A Validation set is a collection of samples that should PASS a model (positive samples) and samples that should FAIL a model (negative samples). The Validation set is an easy and maintainable way of validating a model by giving the user the opportunity to run new tests alongside existing (old) tests in a controlled way. The results of the validation are reported in a PDF report. Validation sets are fully-compliant objects in MIRA Cal P. They are version-controlled and can be signed by multiple levels to prevent undesired modifications. Validation sets are created and edited on the **Validation Set** tab in the **Training Set** editing window.

Regions

Regions allow a user to ignore specific portions of a spectrum. MIRA Cal P allows more than 20 regions of any desired width to be retained while everything that is outside of the regions is ignored (specifically set equal to 0).

ROC/AUC

In order to determine the correct parameters and assess the performance of a model, ROC (Receiver Operating Characteristics) curves are calculated to compare the true positive rate and false positive rate of each model. The ROC curve is summed up by the AUC (Area Under the Curve) value which ranges from 0 to 1.

- An AUC of 1.000 is a perfect model where all positive samples pass and all negative samples fail.
- An AUC of 0.500 is a random model where positive samples pass and fail equally as do negative samples.
- An AUC of 0.000 is an inverted model where all positive samples fail and all negative samples pass.

ROC curves for a model can be accessed and generated from the **[ROC Curves]** button in the **Overview** tab in the **Training Set** editing window.

ModelExpert

ModelExpert leverages the power of ROC curves but eliminates the complexity. With **ModelExpert**, the user simply adds training set and validation set samples then lets the software determine the optimal parameters. The result is a summary window explaining model performance, a PDF report, and a model with the correct parameters.

5.4.4 Verification models (start to finish)

A verification model needs to be planned properly to make sure the test leads to exploitable results. As part of the planning, some questions need to be answered:

- Is the goal to distinguish very dissimilar products or to detect contaminants within the same product?
- Will the products be sampled and tested in vials or tested in situ through a container?

The answers to the questions above will have a large impact on how the model is built and what types of samples are necessary.

Designing a training set and validation set

Collect 3 tests of each variable (discrete sample, container thickness, supplier). Ideally a training set does not include different container materials or different collection optics. These types of variations may result in clusters of data that can cause a traditional PCA model to behave unpredictably.

The validation set is comprised of positive samples which should pass the model and negative samples which should fail the model.

- For the positive samples in the validation set, incorporate unique tests from unique samples that are not in the training set. This is the only way to validate model performance prior to implementation.
- If the model should fail when testing different materials than what is included in the training set, then the negative validation samples should include as many "other" samples as can be collected. If the model should fail when testing contaminated samples, then the validation set should include contaminated samples only. It is unrealistic to expect a PCA model to perform well in both cases.

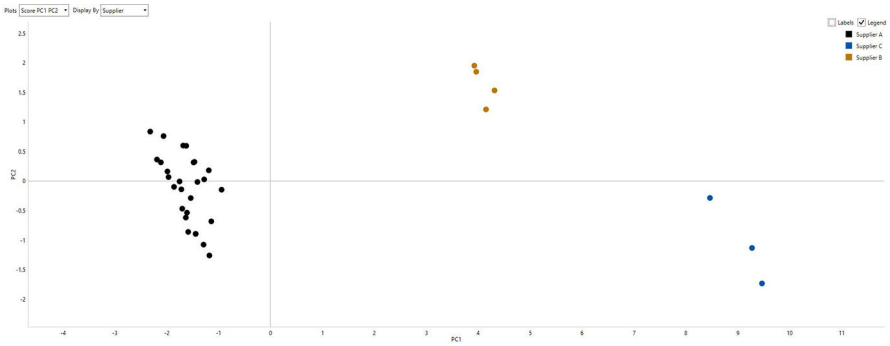
Collecting the training set and validation set samples

1. Build an operating procedure specifically for this training set and validation set according to *"Creating and editing operating procedures", page 31*. The default operating procedure settings (auto-integration, laser power 5, 1 average) should be sufficient unless the sample characteristics are known.
2. Specify the desired collection accessory from the **Smart Tip** drop-down menu. If the samples have barcodes, set up the barcode parsing method to speed up the data entry process. Synchronize this operating procedure to the instrument.
   Using the **Acquire** window, select the desired operating procedure and collect the necessary data for the training set and validation set according to the plan developed above. Training sets must have a minimum of 20 spectra and validation sets must have a minimum of 1 positive and 1 negative.
   During data collection, it is important to complete all known metadata and to name each sample with a unique name. A predetermined nomenclature is helpful to keep track of what has been collected, for example:
   [chemical name]_[lot#]_[supplier]_001
   Where *001* is just a running counter of all the samples collected for that data set. This helps ensure uniqueness even when testing the same sample twice.
   TIP: While the instrument is scanning, the **Acquire** window will stay interactive. Use that time to type in the name of the next sample.
3. Create a new training set according to *"Creating and editing training sets", page 25* using the data that was just collected. Add validation set samples and run **ModelExpert**.
   ModelExpert runtime depends on the size of the training set and validation set. For example, a training set with 20 spectra and a validation set with 10 positive and 10 negative samples will take 10-15 minutes.
4. Review **ModelExpert** results in the popup window. The AUC should be high (1.000 is a perfect score) and the validation set samples should all be correct. Save the validation report and save the training set.
   ModelExpert will not evaluate the model with only 1 principal component. If such a setting is desired, it must be set manually in the training set model as described in *"Creating and editing training sets", page 25*.
5. Now the training set is ready to be added to an operating procedure and tested on the instrument *(see "Creating an operating procedure", page 33)*.

Model Review

In the event that **ModelExpert** is unable to find a perfect setting, try these diagnosis steps:

1. Verify that the samples in the training set are correct.
2. Verify that the samples in the validation set are classified correctly.
3. Review the current model settings by examining the scores and loadings within the training set model from the **Overview** tab. This is where it is invaluable to have samples with good metadata.
4. Use the **Display By** dropdown menu in the plot to color the points in the score plot by:
   Product ID
   Lot ID
   Batch ID
   Container
   Supplier



   This can help determine the source of the problem.
5. Review the model using the **ROC Curves** in the ribbon from the **Overview** tab.
6. Consider building a region mask to isolate areas of the spectrum that are of interest. This is located in the ribbon from the **Overview** tab.
7. Consider 1 Principal Component. This is not recommended for most cases but certain models may require it. **ModelExpert** does not evaluate this case but it can be set manually in the training set model parameters *(see "Creating and editing training sets", page 25)*.

5.4.5 Creating and editing operating procedures

Operating procedures direct the acquisition and evaluation of spectra.

MIRA P/MIRA M-3 runs only on operating procedures that are built in MIRA Cal P. Before using the instrument, users must build operating procedures and synchronize with MIRA P/MIRA M-3. Users can define the acquisition settings *(see table 4, page 31)* as well as what library to match to, what training set to test against, and how to parse out barcodes.

Table 4 Acquisition settings

Acquisition setting	Description
Laser power (level)	The intensity of the laser can be reduced. Choose a value between 1-5. 5 is the maximum. The recommended value is 5. Reasons to lower the laser power are: ▪ Measuring critical materials as explosive or inflammable materials. ▪ Measuring materials with a low melting point. Liquid and solid forms of a compound have different spectra.
Auto integration	The instrument automatically chooses the best Integration time for the current sample.
Integration time (sec.)	The integration time indicates how long a single spectrum is recorded. The integration time is divided into 2 steps. ▪ Laser **ON** to acquire sample spectrum. ▪ Laser **OFF** to acquire reference. The actual time for a measurement is twice the entered value. The maximum integration time is 30 seconds.

Acquisition setting	Description
Averages	If the value is higher than 1, the displayed spectrum is an average of multiple acquisitions. A higher value in this field will lead to a longer measurement time, because more spectra need to be acquired. The maximum number of averages is 10. Example: Enter **5** to have an averaged spectrum of 5 measured samples.
Smart Tip	Select the required attachment to measure your samples. If no dedicated Smart Tip is required, select **Allow all**.

Creating an operating procedure

1 Go to the **Operating Procedure** view.

2 Go to the **Home** tab.

3 Click on **[New]**.

4 Add information about the operating procedure in the **Metadata** tab.

After an operating procedure is saved, its name cannot be changed.

5 Go to the **Acquisition** tab. Select the desired acquisition settings.

6 Go to the **Identification** tab. Select the library to be used for matching from the **Available Libraries**. Click on **[Add]** to move the library to **Identification Libraries**.

In **Match Threshold**, the user can select the minimum Hit Quality Index (HQI). The default value is 0.85.

To remove a library from **Identification**, select the library. Click on **[Remove]**.

If no library is selected, identification will not be performed in the evaluation process.

7 Go to the **Mixture Identification** tab. Select the library to be used for mixture matching from the **Available Libraries**. Click on **[Add]** to move the library to **Identification Libraries**.

To remove a library from **Mixture Identification**, select the library. Click on **[Remove]**.

If no library is selected, mixture identification will not be performed in the evaluation process.

8 Go to the **Verification** tab. Select the training set to be used for verification from the **Available Training Sets**. Click on **[Add]** to move the training set to **Verification Training Sets**.

The user can define a confidence interval between 0.9 and 0.99.

Use **Auto Increment** to analyze a set of containers without having to manually type in the next container number. The user has to define a starting container and an ending container. The system increments the container number automatically.

When the user checks **Auto Increment**, **Rescan Mode** is turned on automatically.

Use **Rescan Mode** to define how many times a container must be scanned to ensure statistical accuracy. The user can set the following parameters to define the conditions for pass and fail of a container.

- Minimum pass
- Maximum fail
- Required rescans

Auto increment and rescan modes are only available on the instrument.

To remove a training set from **Verification Training Sets**, select the training set. Click on **[Remove]**.

If no training set is selected, verification will not be performed in the evaluation process.

9 Go to the **Barcodes** tab. Type in or scan an example of your used barcode content. Define how to extract the needed strings from your barcode.

The following information can be extracted.

- Operating procedure selection: An existing operating procedure will be selected according to the barcode of the sample.

- Lot ID
- Batch ID
- Container

10 Click on **[Save]** to save the operating procedure. If saved properly, the newly created operating procedure will be listed in the **Operating Procedure** view in the **Home** tab.

11 Check the checkbox **Synchronize** to enable synchronization of the operating procedure between MIRA P/MIRA M-3 and MIRA Cal P.

Editing an operating procedure

1 Go to the **Operating Procedures** view.

2 Select an operating procedure. Click on **Edit**.

3 You can edit the following settings.

- **Metadata** (Excluding name which cannot be edited once the OP has been saved)
- **Acquisition**
- **Identification**
- **Mixture Identification**
- **Verification**
- **Barcodes**

4 Click on **[Save]**.

5 Edited operating procedures are synchronized in the same manner as newly created operating procedures.

5.5 Calibration and system suitability

Calibrating MIRA P/MIRA M-3

1. Connect an instrument.
2. Attach a proper calibration standard to the instrument.
3. Place the instrument upright.
4. Click on **Instrument** ▶ **Calibrate instrument**. The calibration may take some time.

   A dialog confirms the success or failure of the calibration.
5. After calibration, the user will be prompted to do a system suitability test. Selecting **[OK]** will automatically run the test. Selecting **[Cancel]** will end the testing.

Performing a system suitability test

A system suitability test is a self-test to demonstrate instrument suitability. Several internal test procedures are performed. For example peak intensity and wavenumber calibration check.

The user can run this test independently of calibration. The test should be run on a daily basis to ensure that the instrument runs as expected. After success or failure of the test, a report can be saved. The report shows details of performed tests.

1. Connect an instrument.
2. Attach a calibration standard to the instrument.
3. Click on **Instrument** ▶ **System Suitability Test**.

   A dialog confirms the success or failure of the test.

   If the system suitability test fails after calibration, refer to the troubleshooting section for more information *"Creating a support log file", page 58*.
4. Select a destination for the report file. Click on **[Save]**.

6 Operation and control

6.1 Acquiring data

Transferring acquired spectra from MIRA P/MIRA M-3 to MIRA Cal P

1 Connect the instrument to MIRA Cal P.

2 Synchronize MIRA P/MIRA M-3 to MIRA Cal P *(see "Connecting MIRA P/MIRA M-3 in MIRA Cal P", page 23)*.

Select **[Synchronize]** from the menu bar.

Samples synchronized to MIRA Cal P appear in the **Sample** view.

Acquiring data with MIRA P/MIRA M-3 connected to MIRA Cal P

1 Connect MIRA P/MIRA M-3 to MIRA Cal P.

2 Go to the **[Samples]** view.

3 Click on **[Acquire]**.

4 Enter the following information

- Operating procedure
  The user can select operating procedures which are created in the software and stored on MIRA P/MIRA M-3.
- Name
  Enter the name of the sample.
- Lot ID, batch ID, container
- Enter the lot ID, batch ID and container manually or scan a barcode to enter them automatically.
  To enter the lot ID, batch ID and container automatically, check the checkbox **Barcode Populate**. Click on **[Scan Barcode]** to start the barcode reader of MIRA P/MIRA M-3.

5 Click on **[Acquire]**.

6 Spectra will be displayed in the **Sample** view.

6.2 Displaying and managing data

6.2.1 Viewing samples

Spectral data view can be used for visual inspection of acquired spectra. Spectral data view can also be used to import and display spectra in the format *.brms or *.srmp.

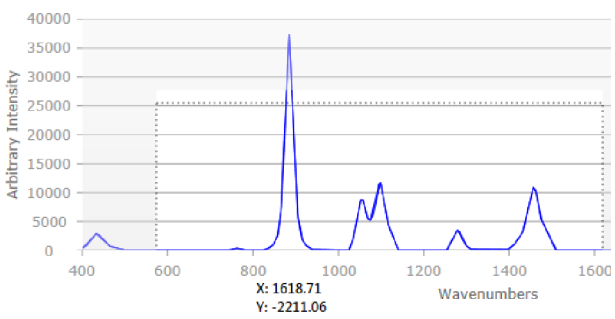
Filter

1 Click on the **Filter** tab. The user can filter large amounts of data by using the filter criteria.

2 Set the desired filter criteria to manage the viewing window data.

3 Click on **[Clear Filters]** to set the filters to default.

Zoom

1 

Click and hold left mouse key, draw a rectangle and release left mouse key.

2 Double-click in spectral data to get back to original size.

6.2.2 Managing sample list folders

1 Select **Sample** view.

2 Folders can be created on the right side of the sample viewing window.

3 To add a sample, select the sample from the sample list. Right click and cut it. Select the desired folder and paste it into the folder.

6.3 Processing a spectrum

Spectral processing does not modify data and should not be used to determine the quality of a sample. This feature is intended as an investigatory tool to help identify samples or containers that fail routine analysis. There is an expected error in the p-value of ±0.001 between instrument and software.

Spectra can be processed or reprocessed by using different methods.

Go to the **Process** tab in the **Sample** view to view different processing options.

Identification

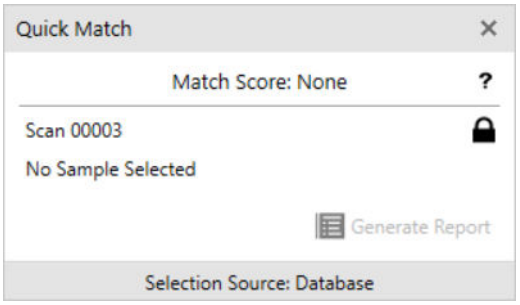
1. Go to the **Identification** area of the **Process** tab.
2. Select the library to match against from the **Library** drop down list.
3. Increase or decrease the number in **Matches** to define the number of results shown.
4. Increase or decrease the number in **Threshold** to define the threshold for the matching. If the user lowers the number, it will increase the chances of false positives.
5. Click on **[Match]** to perform the match with the selected parameters.

Verification

1. Go to the **Verification** area of the **Process** tab.
2. Select the training set to match against from the **Training Set** drop down list.
3. Increase or decrease the **Confidence Interval** to define the limit between pass and fail.
4. Click on **[Match]** to perform the match with the selected parameters.

Quick match

1 Click on **[Quick Match]** to open the **Quick Match** window.

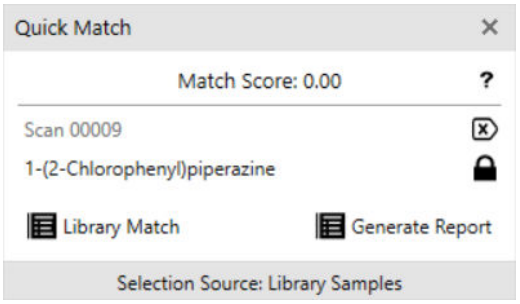


2 The selected spectrum will be shown. Press the icon to lock the active spectrum.

3 Select a different spectrum to display the match score that compares the 2 spectra.

4 Go to the **Library** tab. The **Quick Match** window will stay active.

5 Select a library from the list. Right click on the library and select **View**. Go to the **Library Samples** tab. A library match icon will become active.



6 Click on **[Library Match]** to display the match score as a column in the library list.

7 Click on **[Generate Report]** to generate a match report in .pdf format.

6.4 Audit trail

The audit trail is an automatically generated log of all user activities. The audit trail contains precise logs of user actions, for example date, time, user.

6.5 Generating reports

There are 2 options to generate a sample report. The following 2 procedures describe them. The report looks the same with both procedures. Set parameters for the reports in compliance configuration *(see "Reports tab", page 50)*.

Sample report option 1

1. Select the **Sample** view.
2. Click on the **Reports** tab.
3. Click on either **[Save Summary]**, **[Batch Report]**, **[Save Full]** or **[Save Audit]**.
4. Select a destination for the file. Click on **[Save]**.

Sample report option 2

1. Select a sample. Right click on the selected sample.
2. Go to **Reports**.
3. Select a report format.

There are 2 options to generate a library report. The following 2 procedures describe them. The report looks the same with both procedures.

Library report option 1

1. Select the **Libraries** view.
2. Click on the **Reports** tab.
3. Click on **[Save Full]** or **[Save Audit]**.

4 Select a destination for the file. Click on **[Save]**.

Library report option 2

1 Select a library. Right click on the selected library.

2 Go to **Reports**.

3 Select a report format.

There are 2 options to generate a training set report. The following 2 procedures describe them. The report looks the same with both procedures.

Training set report option 1

1 Select the **Training Sets** view.

2 Click on the **Reports** tab.

3 Click on **[Save Full]** or **[Save Audit]**.

4 Select a destination for the file. Click on **[Save]**.

Training set report option 2

1 Select a training set. Right click on the selected training set.

2 Go to **Reports**.

3 Select a report format.

There are 2 options to generate an operating procedure report. The following 2 procedures describe them. The report looks the same with both procedures.

Operating procedure report option 1

1 Select the **Operating Procedure** view.

2 Click on the **Reports** tab.

3 Click on **[Save Full]** or **[Save Audit]**.

4 Select a destination for the file. Click on **[Save]**.

Operating procedure report option 2

1 Select an operating procedure. Right click on the selected operating procedure.

2 Go to **Reports**.

3 Select a report format.

6.6 Reverting objects

MIRA Cal P offers the opportunity to restore a previous version of an object.

Supported objects are:

- Samples
- Libraries
- Training sets
- Operating procedures

1 Click on **Compliance** ▶ **Revert Objects**

2 Select an object to restore. The version is displayed in the row next to the name.

Different object types can be displayed by switching menu tabs.

3 Click on **[Revert]**.

6.7 Export

Exporting audit trail

1 Click on **Compliance** ▶ **Audit Trail**.

2 Click on **[Save as]**.

3 Select a destination for the file and click on **[Save]**.

Exporting samples

Only samples exported with file type ***.brms** or ***.srmp** can be imported back to MIRA Cal P. These files are encrypted to protect data integrity. ***.brms** is the standard format used in MIRA Cal P.
***.brms** and ***.srmp** contain spectra and metadata such as integration time, matches to any of the used libraries, comments, compliance data and used software and firmware versions.
***.brms** is the recommended file type. ***.srmp** is supported for legacy purposes.

1 Go to the **Samples** view.

2 Select the files to export. Multiple selection is possible.

3 Right click on the sample. Click on **[Save As]**.

4 Select a file type:

- **BRMS format (.brms) / Raman sample**
  This is the default and recommended file type. **BRMS format (.brms)** contains spectra and metadata such as integration time, matches to any of the used libraries, comments, compliance data and used software and firmware versions.
- **SRMP format (.srmp)**
  SRMP format (.srmp) contains spectra and metadata such as integration time, matches to any of the used libraries, comments, compliance data and used software and firmware versions.
- **SPC format (.spc)**
  SPC format (.spc) is optimal for compatibility with third-party spectroscopy software.

- **XML format (.xml)**
  XML format (.xml) is a text format.
- **CSV format (.csv)**
  CSV format (.csv) is a text format.

5 Click on **[Save]**.

Exporting libraries

1 Go to the **Libraries** view.

2 Select the files to export. Multiple selection is possible.

3 Right click on the library. Click **[Save As]**. You can save libraries only as .lrmp file type.

4 Select a destination for the file. Click on **[Save]**.

Exporting training sets

1 Go to the **Training Sets** view.

2 Select the files to export. Multiple selection is possible.

3 Right click on the training set. Click **[Save As]**. You can save training sets as .trmp or .json file type.

4 Select a destination for the file. Click on **[Save]**.

Exporting operating procedures

1 Go to the **Operating Procedures** view.

2 Select the files to export. Multiple selection is possible.

3 Right click on the operating procedure. Click **[Save As]**. You can save operating procedures as .ormp or .json file type.

4 Select a destination for the file. Click on **[Save]**.

6.8 Database backup

Exporting database

Only user roles **Laboratory Manager** and **Administrator** have access to this action.

1 Click on **File** ▶ **Advanced** ▶ **Database** ▶ **Backup**.

2 Select a destination for the file. Click on **[Save]**.

Restoring database

Be aware that the existing MIRA Cal P data is overwritten with the data from the database file.

An existing MIRA Cal P database file must be available in **.litdb** format or **.db** format.

1 Click on **File** ▶ **Advanced** ▶ **Database** ▶ **Restore**.

2 Select the location of the database and the database file to restore. Click **[Open]**.

3 Confirm the restore. Select **[Yes]**.

6.9 Managing

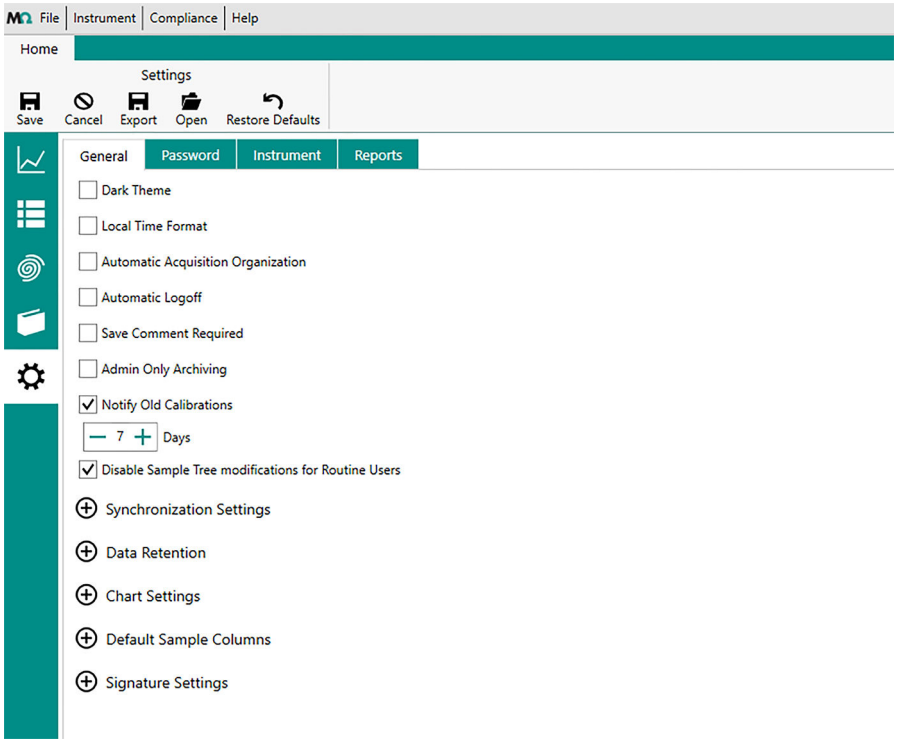
6.9.1 Compliance configuration

Only administrators have access to this area.

Click on **Compliance** ▶ **Compliance Configuration** to open compliance configuration.

General tab

To deploy the same configuration on multiple computers export and import configuration settings. Click **[Export]** in the **Home** tab to export configuration settings. Click **[Open]** to import configuration settings.



General

Dark Theme

Color of the user interface

Local Time Format

Dates and times in the same format as the date and time on the computer (e.g. DD/MM/YYYY vs. MM/DD/YY)

Automatic Acquisition Organization

Samples collected from the Software will go to a dedicated folder that is organized by *Device Name* > *Month Year* > *Date* regardless of the current open folder. If this is turned off, the samples collected from the software will go into the folder that is open. If no folders are open, the software will default to the **Automatic Acquisition Organization** behavior described here.

Automatic Logoff

Automatic logoff after a certain time

Save Comment Required

Force users to write a comment when changing objects.

Admin Only Archiving

Allow only admin users to archive objects.

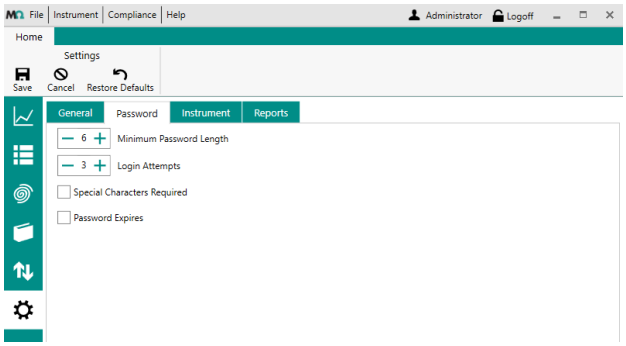
Notify Old Calibrations

Notifies the user when a device has not be calibrated for the set number of days.

Disable Sample Tree

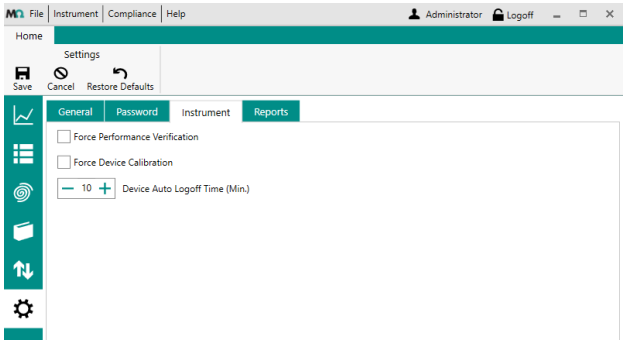
	Modifications for Routine Users: Removes permissions for routine users to modify (create or delete folders, move samples) from the Sample Tree, recommended to use in conjunction with **SmartSync**.
Synchronization settings	**SmartSync** Allows an automatic and configurable sample organization. SmartSync is a predefined folder structure that is generated and maintained on every synchronization. **SmartSync** eliminates the need to manage folders manually. The folders structure can be set by the following variables: ▪ Operating procedure ▪ Day (date of test) ▪ Month ▪ Device name ▪ Serial number ▪ Synchronization time ▪ User ▪ Verification result (pass/fail status) ▪ Batch ID ▪ Container # ▪ Lot ID ▪ Product ID **SmartSync** only applies to tests taken on the device. Tests collected in the Software will be placed inside the current open folder. If no folder is open, a new folder will be created named with the date it is acquired.
Data Retention	Determine a retention period or keep data forever. Defaults is 5 years. A review and backup are required before removing expired data.
Chart settings	Settings regarding the display of spectra. These settings apply for the sample view. Define the same settings by clicking on the sprocket in the sample view.
Default sample columns	Settings regarding the information that is shown in the sample column. These settings apply for the sample view. Define the same settings by right clicking in the sample column.
Signature settings	Modify or remove existing signature reasons. Add new signature reasons.

Password tab



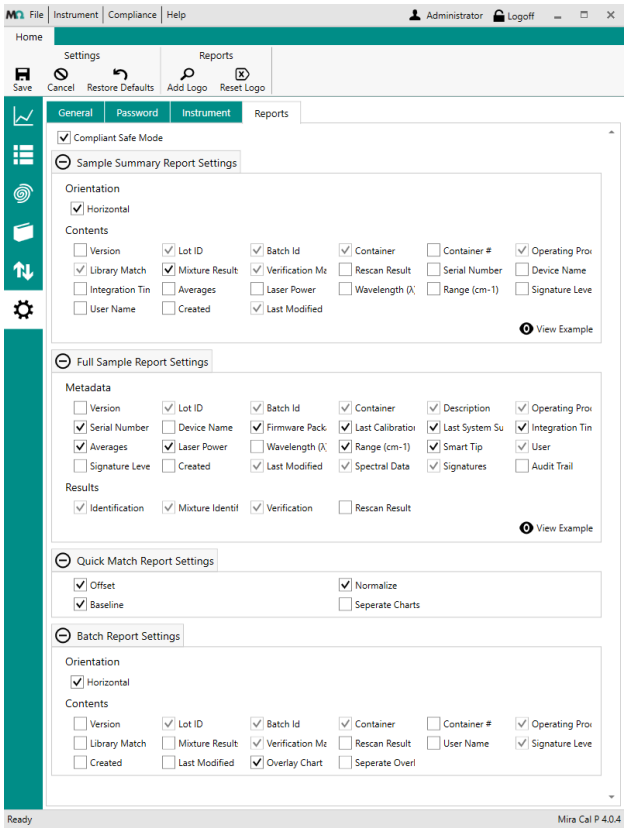
Password	Define settings as minimum lengths of the password, number of possible login attempts, use of special characters and if the password expires.

Instrument tab



Instrument ▶	Define settings regarding performance verification, calibration and automatic logoff time.
Force Performance Verification	If the checkbox is checked, MIRA P/MIRA M-3 must use the CVA for system suitability tests. If the checkbox is unchecked, MIRA P/MIRA M-3 does not require the CVA.

Reports tab



Sample summary report settings	Define the parameters to be shown in the sample summary report.
Full sample report settings	Define the parameters to be shown in the full sample report.
Quick match report settings	Define the parameters to be shown in the quick match report.
Batch report settings	Define the parameters to be shown in the batch report.

6.9.2 Signing objects

In MIRA Cal P the user can sign objects.

Signed objects cannot be edited. If changes are needed, the signature of this object has to be withdrawn first.

Supported objects are:

- Samples
- Libraries
- Training sets
- Operating procedures

The workflow is the same for all objects and described here for an operating procedure.

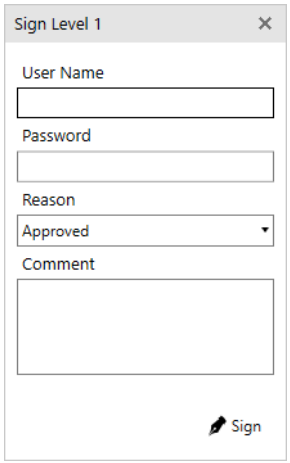
Sign level 1

1 Go to the **Operating procedure** view.

2 Open the **Signatures** tab or right click on the desired operating procedure. Click on **[Sign Level 1]**.

3 Enter login data and choose a reason for signing.

This login is independent of the currently logged in user in MIRA Cal P.



4 Click on **[Sign]**

Signature Level 1 is now displayed in the **Signature** column of the object.

Sign level 2

User group routine user is not allowed to sign on level 2.

A user who signed an object on level 1 is not allowed to sign the same object on level 2. A different user must sign this object.

1 Go to the **Operating procedure** view.

2 Open the **Signatures** tab or right click on the desired operating procedure. Click on **[Sign Level 2]**.

3 Enter login data and choose a reason for signing.

This login is independent of the currently logged in user in MIRA Cal P.

4 Click on **[Sign]**

Signature Level 2 is now displayed in the **Signature** column of the object.

Withdrawing all signatures

User group routine user is not allowed to withdraw signatures.

1 Go to the **Operating procedure** view.

2 Open the **Signatures** tab or right click on the desired operating procedure. Click on **[Withdraw]**.

3 Enter login data and choose a reason for withdrawing.

This login is independent of the currently logged in user in MIRA Cal P.

4 Click on **[Withdraw]**

Unsigned is now displayed in the **Signature** column of the object.

Viewing signatures

View signatures of samples works different, refer to next procedure.

1 Go to the **Operating procedure** view.

2 Open the **Signatures** tab or right click on the desired operating procedure. Click on **[View Signatures]**.

6.9.3 Setting up the user administration

6.9.3.1 Managing users

General information

MIRA Cal P has a build-in user management, which is already active at initial start-up. A general admin account is defined for the first start-up.

Initial user name and password:
User name: admin
Password: Change!

User management is required and cannot be disabled. This means that everyone must use his own user identification to log in. All actions will be logged with that user name.

FDA-compliant settings

To be in compliance with FDA regulations, a user management must be configured. Security settings can be activated according to 21 CFR Part 11 by activating the relevant check boxes. The following conditions will then be complied with:

- A **login with user name and password** is required each time the program is started.
- **User names** must be **unique**. Users cannot be deleted once they have been entered.
- Passwords must be changed after a defined **validity period**.
- **Passwords** must not be **reused**. Last 5 of the expired passwords may not be reused.
- The **number of login attempts** with wrong password is limited. If a pre-defined amount of login attempts with wrong password are performed, the user will automatically be set to **inactive** status (default value is 3).

Define the password settings in compliance configuration *(see "Password tab", page 49)*.

Only administrators have access to the user management area.

Creating a user

1 Go to **Compliance** ▶ **User Management**

2 Click on **[New]** to create a user.

3 Fill in the name. Choose a user group. Enter and confirm the password.

The following user groups exist.

- Routine User
  Connect to the instrument. Acquire and view samples, sign samples on level 1.
- Laboratory manager
  In addition to routine user: Create and manage libraries, training sets and operating procedures. Sign all objects, view and export audit trail, database backup.
- Administrator
  In addition to routine user and laboratory user: Access to user management area. Conduct updates (firmware update, driver for instrument).
- IT Admin
  A limited user level that has permissions to change IT-type settings but not to modify or generate new data. Permissions include:
  - Manage database (location, backups…)
  - Manage users/passwords
  - Manage software configuration (logout time, synchronization settings, custom reports, data export…)

4 The new user has to login to MIRA Cal P and change his start password.

A user will not be synchronized to the instrument until the user has changed the start password to a new password in MIRA Cal P.

Resetting passwords of other users (as an administrator)

1 Go to **Compliance** ▶ **User Management**

2 Select a user in the list and click on **[Edit User]**.

3 Enter new start password twice into the input fields.

4 The affected user has to enter the new start password at his next login attempt. The user has to set a new password afterwards.

A user will not be synchronized to the instrument until the user has changed the provided start password to a new password in MIRA Cal P.

Changing own password

1 Go to **Compliance** ▶ **Change Password**

2 Enter old password.

Enter new start password twice into the input fields.

The new password is active for the next MIRA Cal P login.

Disabling/enabling users

1 Go to **Compliance** ▶ **User Management**

2 Select a user in the list.

3 Enable or disable the checkbox **Enabled**.

Affected users won't have access to MIRA Cal P any longer

A user will not automatically have to enter a new password after his status has changed from disabled to re-enabled. If a password change is needed due to your company policy, the administrator has to manually reset the password of the locked user in a second step.

6.9.3.2 Permissions for user levels

Table 5 x = Yes, o = can be enabled

Action	Routine user	Lab manager	IT	Administrator
Synchronize device	x	x	x	x
Add user to device	x	x		x
Take tests	x	x		x
Open samples (encrypted)	x	x		x
Save samples	x	x		x
Average multiple tests	x	x		x
Reprocess tests	x	x		x
Search and filter samples	x	x		x
Generate reports	x	x		x
Data Set Acquisition		x		x
Group Viewer	x	x		x

Action	Routine user	Lab manager	IT	Administrator
Create and edit libraries		x		x
Sign libraries		x		x
Create and edit training sets		x		x
Sign Training sets		x		x
Manage operating procedures		x		x
Sign operating procedures		x		x
Sign level 1	x	x		x
Sign level 2		x		x
Withdraw signatures		x		x
Revert objects to prior version		x		x
Modify sample browser (folders)	o	x		x
View limited Audit Trail (per object only)	x	x		x
View full Audit Trail		x	x	x
Run calibration and system suitability test	x	x	x	x
View system suitability test archive	x	x	x	x
Change own password	x	x	x	x
Manage users			x	x
Compliance configuration			x	x
Update software and firmware			x	x
Backup database		x	x	x
Restore database			x	x
Reset database			x	x
Change language of SW			x	x
View device information	x	x	x	x
Set device permissions			x	x
Execute script			x	x
Create support file	x	x	x	x

Compliance Configuration includes (but not limited to):

- Time format
- Password policy
- Enforcing save comments
- Auto-logoff time
- Synchronization settings
- Report settings
- Signature settings
- Default sample columns
- Data retention period and settings
- Calibration period
- Import custom XSLT reports

Other functions:

- Export configuration settings
- Import configuration settings
- Restore default configuration settings

7 Malfunctions and troubleshooting

7.1 Creating a support log file

With the help of this function, a log file can be created. In a support case, the created log file can be sent to your regional Metrohm representative.

A calibration standard must be attached.

Creating a support log

The support file is adaptive:

- If an instrument is attached, it will collect instrument data.
- If no device is attached, it will only collect PC data.

1 Click on **Help** ▶ **Create Support File**.

A log file is created. This may take some time.

2 Select a destination for the file. Click on **[Save]**.