Mira Cal 3.1

Tutorial

8.105.8060EN / 2017-07-01

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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.

Table of contents

1 Overview

1.1 Program description

Mira Cal software is used together with the Metrohm Instant Raman Analyzers Mira M-3.

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

Synchronization between Mira instruments and Mira Cal software

With the help of a synchronization workflow, all needed data is synchronized between Mira Cal software and M-3 instruments.

Synchronizing M-3 instruments to Mira Cal 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 trial are saved to the database.

More than one instrument 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 software, two evaluation options are available:

- Identification of samples:
  The measured spectrum of a substance is compared with existing spectra in a library. The best match is reported *(see Chapter 1.3, page 2)*.
- Verification of samples:
  This option is used to check if the measured substance corresponds to what was expected *(see Chapter 1.4, page 3)*.

It is possible to combine both options as well.

Pharma compliant software

- User management
- Electronic signatures of objects
- Audit trail

1.2 Operating procedures

All parameters affecting the acquisition and evaluation of spectra are defined in operating procedures. This ensures that measurement is done in a reproducible and well defined way. Operating procedures are not dependent on a specific instrument, they can be transferred between instruments.

In Mira Cal software, two evaluation options can be linked to an operating procedure:

- Libraries *(see Chapter 3.3.2, page 18)*
- Training Sets *(see Chapter 3.3.3, page 19)*

How to create an operating procedure: *(see Chapter 3.3.1, page 11)*.

1.3 Identification of samples with libraries

The measured spectrum of a substance is compared with existing spectra in a library.

Typical application for identification analysis: Identify and differentiate between salts such as carbonates, phosphates, and sulfates (**without** prior knowledge/expectation about the samples identity).

Creating a library

Before sample evaluation, the user needs to create a "Library" in Mira Cal software, which will then be used for identification of samples. Identification libraries are generated in Mira Cal from spectra from each of the samples you want to identify among. No other reference values are needed.

Define match score limit:

When a library is linked to an operating procedure, a match score limit can be configured. The value between 0 and 1 defines the threshold for the library match. For example choosing a value near "1": The instrument will only give an identification result if the measured spectrum matches very exact to the library spectrum.

Purchase commercial Libraries

In addition to user libraries (acquired by the user himself), Metrohm offers different sets of ready-to-use libraries.

How to activate this libraries: *(see Chapter 3.3.4, page 20)*.

Identification of a substance

When analyzing a sample, the sample spectrum will be compared to all the spectra in the identification library. The measured sample will be iden-

tified as one of the library samples and displayed as "Identification Result". If there is no match of the sample to a library, no match will be displayed.

1.4 Verification of 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 like raw material verification before use (**with** prior knowledge/expectation about the samples identity).

Creating a training set

Before sample evaluation, the user needs to create a "training set" in Mira Cal software, which will then 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. It is of high importance that these samples are representative of 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 of the verification. For statistical purposes it is thereforerecommended to measure a minimum of 20 samples.

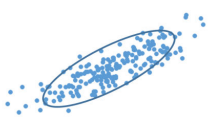
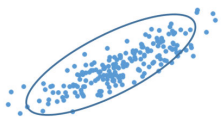
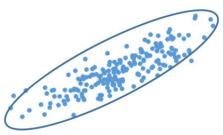
Define Confidence Interval:

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 lead to less false negatives (that means samples actually belonging to the population being rejected) and increase the probability of false positives.

A low confidence interval will lead to less false positives (that means incorrectly accepting a wrong substance as pass result).

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.

Verification of 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.

1.5 Product versions

The products are available in the following versions:

Table 1 Product versions

Order number	Designation	Version feature
6.0607.1010	Mira Cal software	Version 3.1

1.6 About the documentation

NOTE

Please read through this documentation carefully before putting the product into operation.

The documentation contains important information and warnings which you must follow in order to ensure safe operation of the product.

Symbols and conventions

The following icons and formatting may appear in this documentation:

*(5-**12**)*	**Cross-reference to figure legend** The first number refers to the figure number, the second to the product part in the figure.
1	**Instruction step** Carry out these steps in the sequence shown.
Method	Designations for names of parameters, menu items, tabs and dialog windows in the software.
File ▸ New	Menu or menu item
Work area / Properties	Menu paths in order to arrive at a particular position in the software.
[Next]	**Button** or **key**

1.7 Additional information - hardware manuals

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

- Mira M-3 User Manual: 8.924.8010EN

2 Installation

2.1 System requirements

Processor	Pentium 4 equivalent or higher
Operating system 32 or 64 bit version of:	▪ Windows 10 ▪ Windows 8.1 ▪ Windows 8 ▪ Windows 7
Screen resolution	Resolution 1024 x 768 or higher, EGA equivalent or higher
RAM	All operating systems: 1 GB minimum; 4 GB recommended
Hard disk capacity	Minimum 100 GB; 500 GB recommended
USB connectors	USB 2.0, powered port recommended
Mouse	Required, USB, PS/2 style, or wireless
Keyboard	Compatible keyboard using USB / PS/2, or similar connection
Printer compatibility	Must be connected to one of the following: ▪ USB printer ▪ Network printer within immediate work area ▪ Alternative print connection, including parallel, or other reliable methods (A test page should be printed to verify correct operation).
System backup	Network or CD backup required for data archiving.

2.2 Install the software

Install the software

NOTE

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

NOTE

Make sure, the used system fulfils the system requirements. *(see Chapter 2.1, page 6)*

1 Double-click on Installer file.

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

NOTE

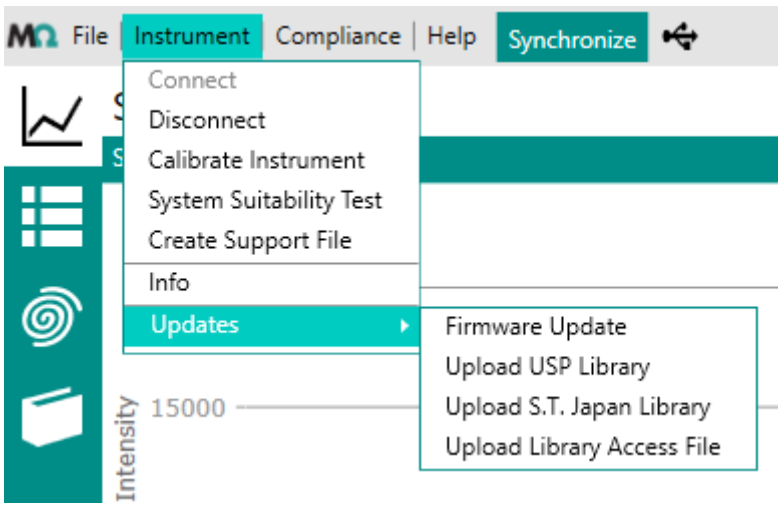
If missing, additional third party software will be installed as well.

2.3 Update firmware

NOTE

After a Firmware update, the instrument must be calibrated again. Information regarding calibration can be found here *(see Chapter 3.4.1, page 20)*.

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.

NOTE

Instrument status including firmware version can at any time be displayed. Detailed Information can be found here *(see Chapter 4.4.1, page 25)*.

3 Initial start-up

3.1 Start Mira Cal

NOTE

Initial User Name and Password

User Name: admin

Password: Change!

1 Double-click on , to start the program.

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

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

3.2 Establish connection

NOTE

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

Physically connect the instrument to the host

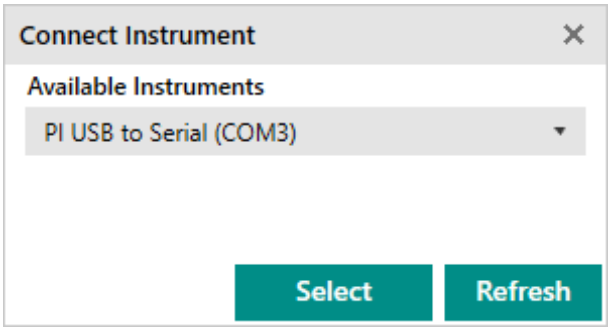
1 Connect the instrument to the computer using the USB Mini-B cable.

Instrument turns on. Wait a moment for the instrument to be ready. Login screen appears on the instrument.

Connect the instrument in Mira Cal software

1 In Mira Cal software click on **Instrument** ▸ **Connect**.

2



The name of the instrument driver is listed in the drop-down list „Available Instruments“.

Select the desired instrument and click on **[Select]**.

NOTE

If the instrument is not listed, click on **[Refresh]** again.

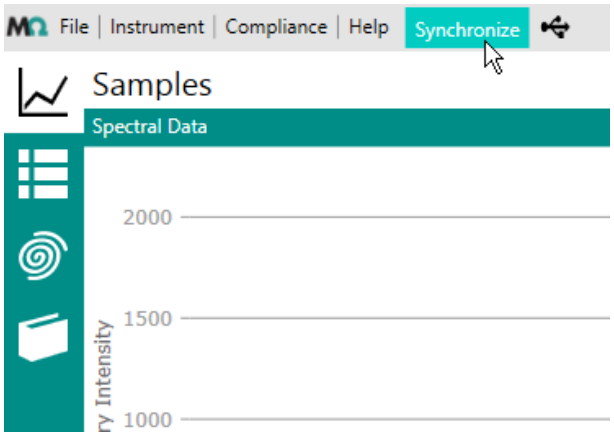
Make sure the instrument is turned on. It will not be listed if turned off.

NOTE

A successful connection is indicated by the icon in the menu bar of Mira Cal software.

The text "Connected" is displayed on the screen of the instrument.

Initial synchronization of the instrument

1 

Click on **Instrument** ▸ **Synchronize** to transfer data (for example samples or operating procedures) between the instrument and Mira Cal software.

Disconnect the instrument

1 Click on **Instrument** ▸ **Disconnect**, to disconnect the instrument.

3.3 Configuration

3.3.1 Create an operating procedure

What is an operating procedure? *(see Chapter 1.1, page 1)*

1 Go to "Operating Procedures" section.

2 Click on **[New]**.

3 Fill in the fields of the tab "Info".

Input field	Description
Operating Procedure Name	Name of the operating procedure. The name must be unique for every existing operating procedure in the database. If the operating procedure was saved for the first time, this value cannot be changed anymore. Required value.
Sample Name	This value will be displayed as default for samples measured with this operating procedure. Optional value.
Description	Space for adding a description to the operating procedure. Optional value.

4 Go to tab "Acquisition".

5 Fill in the fields of the tab "Acquisition".

Input field	Description
Laser Power (level)	The intensity of the laser can be reduced. Choose a value between 1-5, 5 is maximum. Recommended value is 5. Reasons to lower the Laser Power are: ▪ Measuring critical (explosive, inflammable) materials ▪ Measuring materials with a low melting point (liquid and solid forms of a compound will have different spectra)

Input field	Description
Integration Time (sec.)	The integration time indicates how long a single spectrum is recorded. Integration Time is divided into two steps: ▪ Laser ON to acquire sample spectrum. ▪ Laser OFF to acquire reference. Actual time for a measurement is twice the entered value.
Auto Integration	If selected, the instrument automatically chooses the best Integration time for the current sample.
Averages	If the value is higher than "1", the displayed spectrum is an average of multiple acquisitions. For example: Enter "5" to have an averaged spectrum of 5 measured samples. A higher value in this field will lead to a longer measurement time, because more spectra need to be acquired.
Smart Tip	Select the required attachment to measure your samples. If no dedicated Smart Tip is required, "Allow all" can be selected. What is a Smart Tip? *(see Chapter 4.2, page 23)*.

6 Go to tab "Evaluation".

7 Choose the form of Evaluation for the operating procedure.

Field	Description
Verification	Activate checkmark for verification of samples with a training set. A training set must be available and selected. **Confidence interval:** Select a value between 0-1 What is a training set *(see Chapter 1.1, page 1)*? How to create a training set *(see Chapter 3.3.3, page 19)*?
Identification	Activate checkmark for identification of samples with a library. A library must be available and at least one must be selected. **Match Score Limit:** Select a value between 0-1. Match Score Limit defines the threshold for the library. What is a library? *(see Chapter 1.1, page 1)*? How to create a library *(see Chapter 3.3.2, page 18)*?
Mixture Identification	Activate checkmark for identification of samples with a library. A library must be available and at least one must be selected. What is a library? *(see Chapter 1.1, page 1)*? How to create a library *(see Chapter 3.3.2, page 18)*?

8 Go to tab "Barcodes".

9 Type in or scan (with button **[Scan Barcode]**) an example of your used barcode content. Define how to extract the needed strings from your barcode.

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

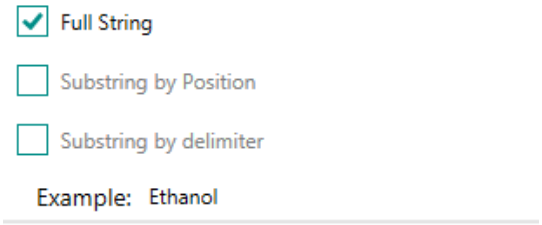
NOTE

If nothing is selected, always the full content of the barcode is read.

This are the possible ways to extract data:

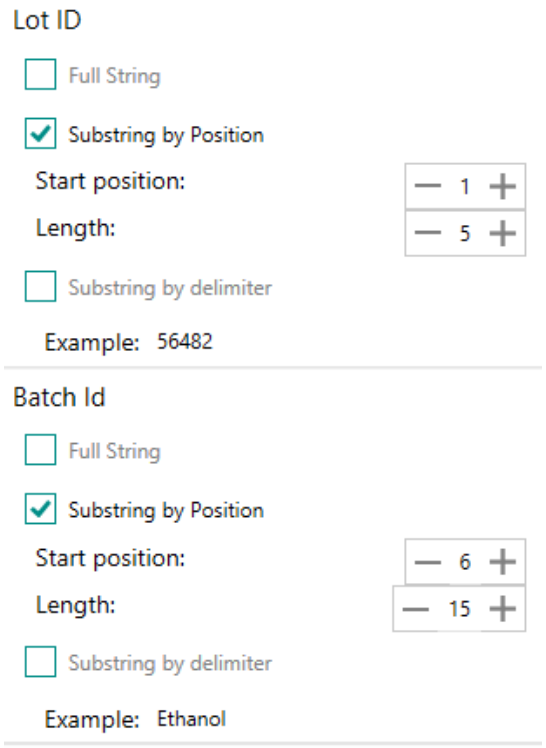
- **Use full string**
  Example for an extraction of the full information of the barcode:

Respective settings to be entered in Mira Cal software:



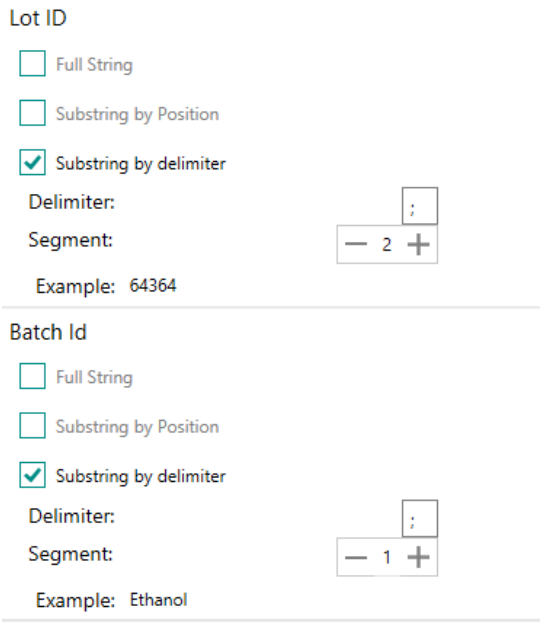
- **Use substring by position**
  Example for an extraction of information by position:

Respective settings to be entered in Mira Cal software:



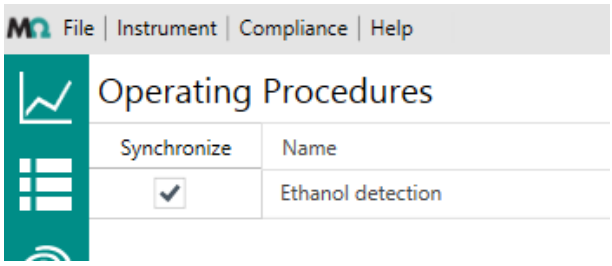
- **Use substring by delimiter**
  Example for an extraction of information divided by a special character (delimiter):

Respective settings to be entered in Mira Cal software:



10 Click on **[Save]** to save the whole operating procedure.

11 Make sure the checkmark to sychronize the operating procedure is enabled.



12 Synchronize the instrument with Mira Cal software to upload the operating procedure to the instrument. The Instrument must be connected.

Click on **Instrument ▸ Synchronize**

3.3.2 Create a library

What is a library? *(see Chapter 1.1, page 1)*

Create a library

Needed spectra have to be acquired beforehand and must be synchronized to Mira Cal software.

1. Go to "Libraries" section.
2. Click on **[New]**.
3. Add library information.

   If the library was saved for the first time, the library name cannot be changed anymore.
4. Go to tab "Samples".
5. Click on **[Add Samples]**.
6. Select samples, multiple selection with CTRL/SHIFT key.
7. Click on **[Add]**.
8. Click on **[Save]** to create the new library.

   The new library is now displayed in the list of libraries.
9. Create or edit an operating procedure and link the created library to the operating procedure. *(see Chapter 3.3.1, page 11)*

Edit an existing library

NOTE

Only unsigned libraries can be edited. Withdraw all signatures if you want to edit an existing library *(see Chapter 4.11.1, page 36)*.

1. Go to "Libraries" section.
2. Select a library and click on **[Edit/View]**.

3 Perform changes:

- More samples can be added: Click on **[Add Samples]**.
- Remove samples: Select samples to remove and click on **[Remove]**.

4 Click on **[Save]**

A new version of the library is created.

Information how to revert an object is described here *(see Chapter 4.10, page 35)*.

3.3.3 Create a training set

What is a training set? *(see Chapter 1.1, page 1)*

NOTE

The software requires a minimum of 6 samples to create a training set model, but for statistical purposes a minimum of 20 samples is recommended for each training set.

Tips for building a good training set:

- Minimum 20 samples (more is ideal).
- It is recommended, for most samples, to enable auto integration time feature for collecting training set data.
- If possible, collect data from multiple batches/suppliers of material.
- Move to different positions on the sample in between measurements.
- If a sample has poor signal-to-noise, averaging at least 5-10 spectra is recommended.
- If using vials for analysis, it is recommended that you collect data from several different vials.

Needed spectra have to be acquired beforehand and must be synchronized to the database of Mira Cal software.

1 Go to "Training Set" section.

2 Click on **[New]**.

3 Fill in the fields of the tab "Acquisition".

Sample Name: The name of the expected substance as it will be displayed after acquisition (in reports for example).

If the training set was saved for the first time, the name cannot be changed anymore.

4 Go to tab "Samples".

5 Click on **[Add Samples]**.

6 Select samples, multiple selection with CTRL/SHIFT key.

7 Click on **[Add]**.

8 Click on **[Save]** to save the whole training set.

9 Create or edit an operating procedure and link the created training set to the operating procedure. *(see Chapter 3.3.1, page 11)*

3.3.4 Activate commercial libraries

1 Contact your Metrohm representative to buy an activation file.

You will be provided with an activation file.

2 Login to Mira Cal software as an administrator.

3 Connect with an instrument *(see Chapter 3.2, page 9)*.

4 Click on **Instrument ▸ Updates ▸ Upload Library Access File**

5 Select the destination of your file and click on **[OK]**.

3.4 Calibration

3.4.1 Calibrate an instrument

1 Connect an instrument.

2 Attach a proper Calibration Standard to the instrument *(see Chapter 4.2, page 23)*.

3 Click on **Instrument ▸ Calibrate instrument**. The calibration may take some time.

A dialog window confirms the successful calibration.

Possible reasons for a failed calibration:

- Expired Calibration Standard

4 After successful calibration, the System Suitability Test will automatically be performed.

3.4.2 Perform a system suitability test

A system suitability test is a self-test to demonstrate instrument suitability. In the background several internal test procedures are performed.

The user can run this test on a daily basis to be sure that the instrument runs as expected.

After successful test, a report lists the result of performed tests.

1 Connect an instrument.

2 Attach a proper calibration standard to the instrument.

3 Click on **Instrument ▸ System Suitability Test**.

A dialog window displays the overall test result: passed or failed.

If the test fails, calibrate the M3. The system suitability test will then automatically be performed.

Details about failed tests are displayed in the report file.

If the system suitability test fails after calibration, refer to the troubleshooting section for more information.

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

4 Operation and control

4.1 Menu sections

NOTE

Depending on the user role, not all menu sections are visible *(see Chapter 4.11.4, page 43)*.

Mira Cal software has different program functions. Click on the corresponding menu item symbol in the vertical bar on the left to change the program function.

The menu section symbol for the opened program function is shown in white background. The symbols for the other program functions in green.

The menus, tool bars and content of the main window depend on the menu section currently opened.

Menu item "Samples"

- View sample information.
- Import and export acquired spectra to and from a local drive.
- Sign samples.

Menu item "Libraries"

- Create and edit libraries.
  Only available for users with the role laboratory manager or administrator.
- Sign libraries.
  Only available for users with the role laboratory manager or administrator.

Menu item "Training Sets"

- Create and edit training sets.
  Only available for users with the role laboratory manager or administrator.
- Sign training sets.
  Only available for users with the role laboratory manager or administrator.

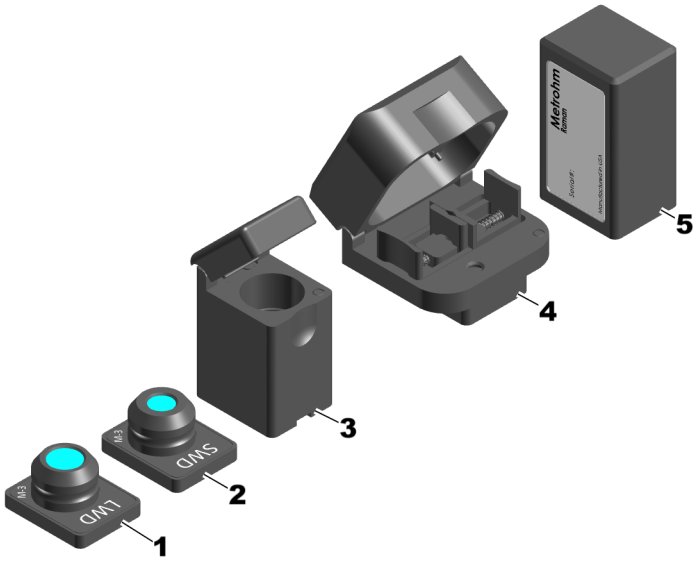
Menu item "Operating Procedures"

- Manage your operating procedures.
  Only available for users with the role laboratory manager or administrator.
- Sign operating procedures.
  Only available for users with the role laboratory manager or administrator.

4.2 Smart tips for Mira instruments

The following smart tips are available.

Smart tips are attached to the instrument with magnetic connectors. The smart tips contain a memory chip so that they can be identified by the instrument. Due to its design, smart tips cannot be attached in a wrong position.



1 Long distance attachment lens (LWD)
A long distance lens for point and shoot measurement with laser class 3.

The focal point is approximately **8 mm** from the top of the lens.

The LWD lens is used for samples in thick-walled bottles.

2 Short distance attachment lens (SWD)
A short distance lens for point and shoot measurement with laser class 3.

The focal point is approximately **0.85 mm** from the top of the lens.

The SWD lens is used for samples with direct contact or in thin plastic bags.

3 **Vial holder**
The Vial holder is used for samples in glass vials.

Safety switch mechanism allows measurement with laser class 1. Laser stops if housing is opened.

4 **Tablet holder**
A spring-loaded holder helps to mount and position the sample. The tablet holder is designed such that different tablet or capsule shapes can be used.

Safety switch mechanism allows measurement with laser class 1. Laser stops if housing is opened.

5 **Calibration standard**
The calibration standard contains an ASTM 1840 reference sample and is needed for the calibration of the instrument.

4.3 Data acquisition

4.3.1 Data acquisition with instrument

Acquire data

NOTE

Refer to instrument user manual for detailed description of the following steps.

1. If any changes were made, sychronize instrument with Mira Cal software to upload operating procedures, user accounts.
2. Disconnect instrument from Mira Cal software.
3. Login to instrument.

   Credentials have to be configured beforehand in Mira Cal software *(see Chapter 4.11.4, page 43)*.
4. Select operating procedure.
5. Acquire spectra.

Transfer acquired spectra from instrument to Mira Cal software

1. Connect instrument to Mira Cal software.

2 In Mira Cal software select **Instrument** ▸ **Synchronize**.

Instrument synchronizes and samples are listed in Mira Cal software.

4.3.2 Data acquisition with software

Acquire data

NOTE

Refer to instrument user manual for detailed description of instrument-specific tasks.

1 Connect an instrument.

2 Go to "Operating Procedures" section.

3 Click on **[Acquire]**.

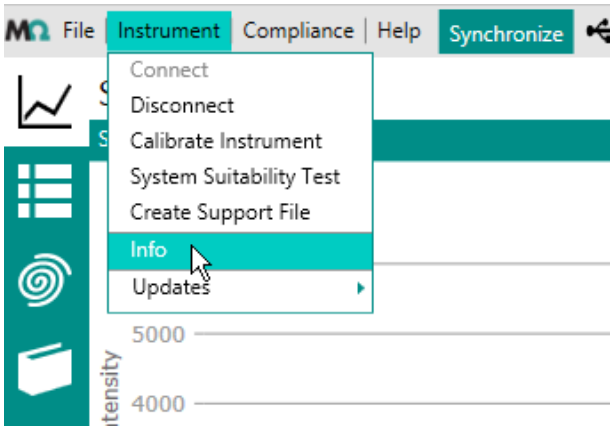
4 Select an operating procedure, enter meta data and click on **[Acquire]**.

Data acquisition starts and a laser warning icon is displayed in Mira Cal during acquisition.

4.4 Display and control data

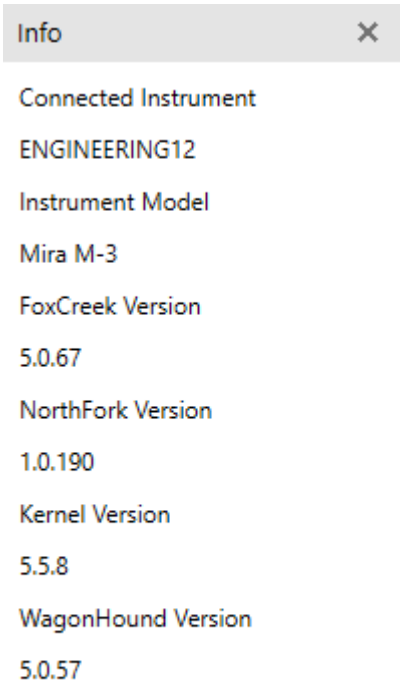
4.4.1 Display instrument information

1 Connect to an instrument

2 

Click on **Instrument ▸ Info**

Instrument information will be displayed.



4.4.2 View samples

Spectra view can be used for visual inspection of acquired spectra. Spectra View can also be used to import and display spectra in the format *.srmp. = "Protected sample".

Zoom

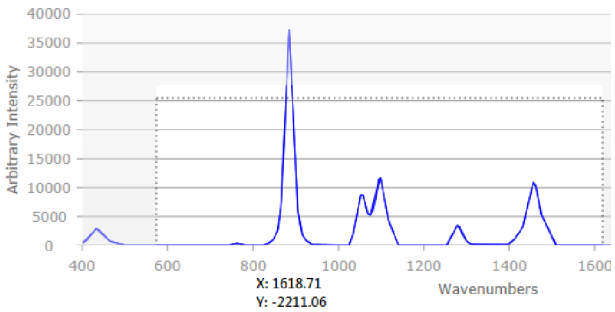
1. Click and hold in Spectra view with left mouse key.
2. 

Figure 1 Zoom

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

3 Double-click in Spectra view to get back to original size.

Detail Pane

1 

Figure 2 Selection "Detail Pane"

Mark check box "Detail Pane".

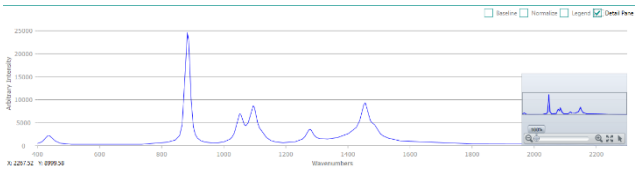
2 

Figure 3 Window "Zoom"

The opening window zooms into displayed spectrum.

NOTE

The same zoom can be used in different areas of a spectrum.

3 Click on to get back to original size.

Normalize spectra

Spectra can be selected to display the names.

NOTE

A multiple selection of spectra with **[CTRL/SHIFT]** is possible.

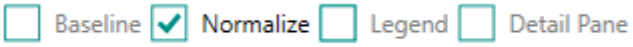
1 

Figure 4 Selection "Normalize"

Mark Check box "Normalize" that spectra can be normalized.

Display legend

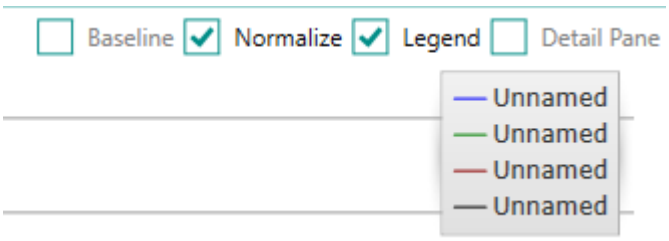
1 

Figure 5 Selection "Legend"

Mark Check box "Legend" to display the legend.

4.4.3 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. Recording an audit trail is important for compliance with FDA Guidance 21 CFR Part 11 when using PC programs.

Display audit trail

1 Click on **Compliance ▸ Audit Trail**

Audit trail opens and all entries are displayed.

Export options are explained here *(see Chapter 4.8, page 31)*.

4.5 Log in

NOTE

Initial User Name and Password

User Name: admin

Password: Change!

This initial user will not be synchronized to the instrument.

NOTE

Login dialog is displayed automatically when starting Mira Cal software.

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

4.6 Log off

User must be logged in.

1 Click on **[Logoff]** in the top-right corner of Mira Cal software.

NOTE

Automatic Logoff

If the automatic logoff is activated, the user will automatically be logged off after a defined time without any user interaction *(see Chapter 4.11.3, page 41)*.

4.7 Reports

4.7.1 Generate reports

In Mira Cal software the user can generate different PDF reports.

- All generated files are secured PDFs.
- Printout is possible.

Sample report

1 Go to "Samples" section.

2 Right click the desired sample in the list and click on **[Information]** in the dialog menu.

3 Click on the button **[Generate Report]**.

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

5 If needed, print out the PDF file.

Operating Procedure report

1 Go to "Operating Procedure" section.

2 Right click the desired Operating Procedure in the list and click on **[Generate Report]** in the dialog menu.

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

4 If needed, print out the PDF file.

Summary Report

1 Go to "Samples" section.

2 Select one or more Samples in the list. Multiple selection is possible with CTRL/SHIFT key.

3 Click on the button **[Summary Report]**.

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

5 If needed, print out the PDF file.

Batch Report

1 Go to "Samples" section.

2 Select one or more Samples in the list. Multiple selection is possible with CTRL/SHIFT key.

3 Click on the button **[Batch Report]**.

4 Select a batch and click on **[Generate Report]**.

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

6 If needed, print out the PDF file.

4.8 Exporting

Exporting Audit Trail

1. Click on **Compliance** ▸ **Audit Trail**
2. Click on **[Export]**
3. Choose a file type. CSV (as .txt) and MS Excel (as .xlsx) are available.
4. Select a destination for the file and click on **[Save]**.

Archiving Audit Trail

Audit Trails can be archived as a secured pdf file.

1. Click on **Compliance** ▸ **Audit Trail**
2. Click on **[Archive]**
3. Select if you want to keep the Audit Trail logs listed in Mira Cal. Click on **[Yes]** or **[No]**.

> **NOTE**
>
> If you click **[No]**, the Audit Trail entries are no longer displayed in the Audit Trail within Mira Cal Software.

4. Select a destination for the file and click on **[Save]**.
5. If needed, print out the PDF file.

Exporting Samples

NOTE

Only samples exported with file type **PROTECTED SAMPLE (.srmp)** can be imported back to Mira Cal software.

This is the standard format used in Mira Cal software. Besides the spectra, it contains metadata, such as integration time, matches to any of the used libraries, comments, compliance data and used software and firmware versions.

1. Go to "Samples" section.
2. Select the files to export. Multiple selection is possible.
3. Select a file type:
   - **PROTECTED SAMPLE (.srmp)**
     This is the standard format used in Mira Cal software. Besides the spectra, it contains metadata, such as integration time, matches to any of the used libraries, comments, compliance data and used software and firmware versions.
   - **RAMAN (.rmn)**
     Besides the spectra, it contains metadata, such as integration time, matches to any of the used libraries, comments and used software and firmware versions.
   - **GRAMS SPC format (.spc)**
     A widely used file format in spectroscopy. It is however lacking some of the functionality of .rmn files, so it is recommended to use it only for data transfer to other software.
   - **ASCII (.txt)**
     A very versatile data format, readable by humans and various software alike. It is typically used when spectra shall be exported to other software packages such as *Excel*, *MATLAB* und *R*.
4. Click on **[Export]**.
5. Select a destination for the file and click on **[Save]**.

Exporting Libraries

1. Go to "Libraries" section.
2. Select the files to export. Multiple selection is possible.
3. Click on **[Export]**.
4. Select a destination for the file and click on **[Save]**.

Exporting Training Sets

1. Go to "Training Sets" section.
2. Select the files to export. Multiple selection is possible.
3. Click on **[Export]**.
4. Select a destination for the file and click on **[Save]**.

Exporting Operating Procedures

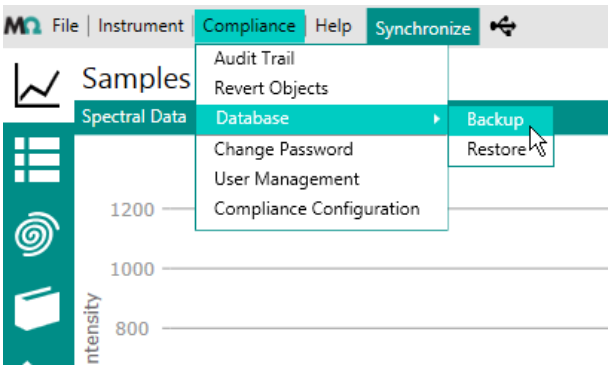
1. Go to "Operating Procedures" section.
2. Select the files to export. Multiple selection is possible.
3. Click on **[Export]**.
4. Select a destination for the file and click on **[Save]**.

4.9 Database backup

Exporting Database

NOTE

Only user role Lab Manager and Administrator have access to this action.

1 

Click on **Compliance** ▸ **Database** ▸ **Backup**

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

Restoring Database

NOTE

Only user Administrator has access to this action.

NOTE

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

An existing Mira Cal database file must be available. File format: **DATABASE FILE .db**.

1 Click on **Compliance** ▸ **Database** ▸ **Restore**

2 Agree to the question that existing data from Mira Cal will be overwritten.

3 Select the destination of the database file and click on **[OK]**.

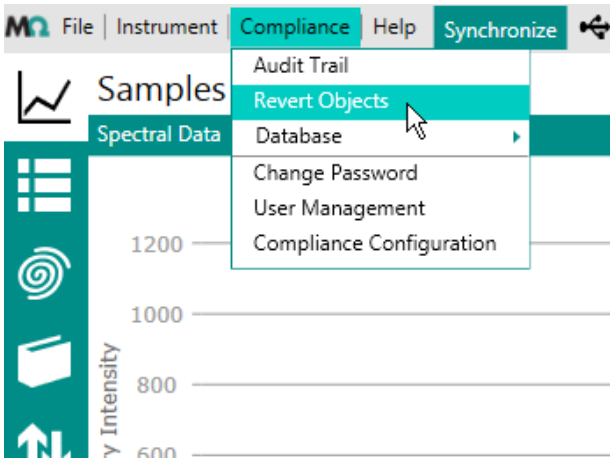
4.10 Reverting objects

Mira Cal software 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]**.

4.11 Manage

4.11.1 Signing objects

In Mira Cal software the user can sign objects.

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

Supported objects are:

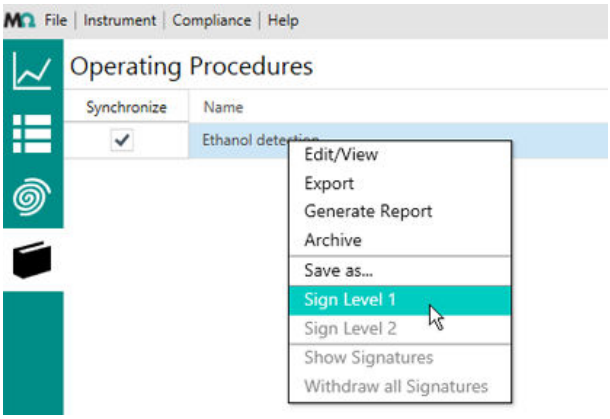
- Samples
- Libraries
- Training Sets
- Operating Procedures

The workflow is the same for all objects and described here in detail for object type Operating Procedure only.

Sign Level 1

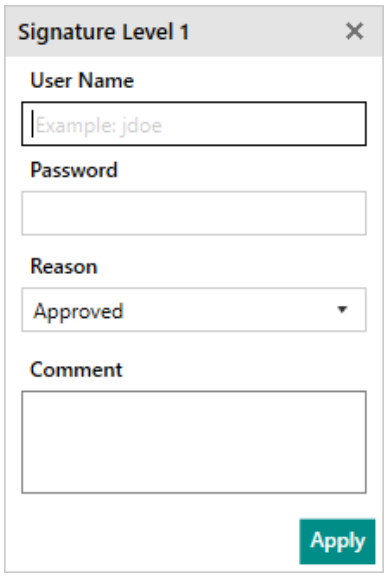
1 Go to "Operating Procedures" section.

2 Right click on the desired operating procedure and click on **[Sign Level 1]**.



3 Enter Login and choose a reason for signing.

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



4 Click on **[Apply]**

"Signed on Level 1" is now displayed in the "Signature" row of the object.

Sign Level 2

NOTE

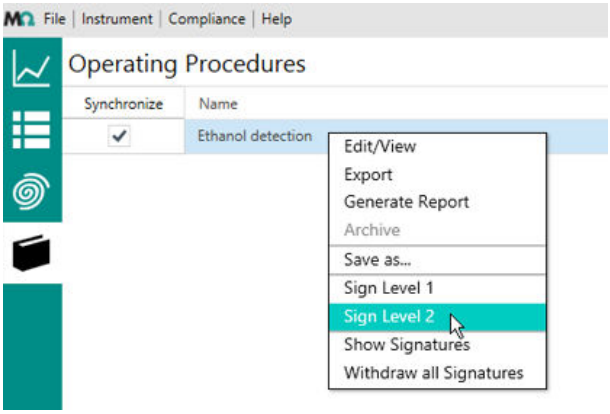
User group "routine user" is not allowed to sign on level 2.

NOTE

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.

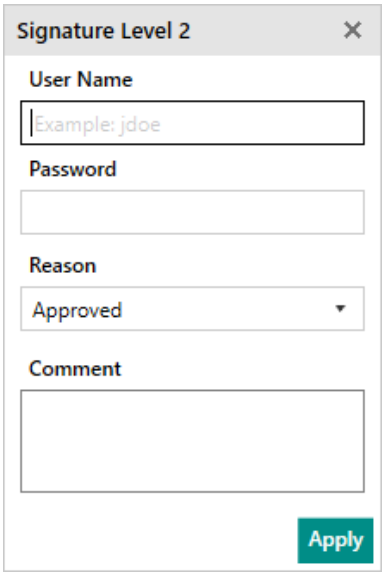
1 Go to "Operating Procedures" section.

2 Right click on the desired Operating Procedure and click on **[Sign Level 2]**.



3 Enter Login and choose a reason for signing.

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



4 Click on **[Apply]**

"Signed on Level 2" is now displayed in the "Signature" row of the object.

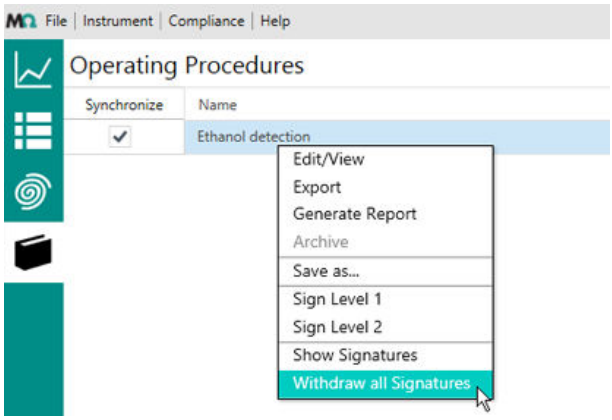
Withdraw all Signatures

NOTE

User group "routine user" is not allowed to withdraw signatures.

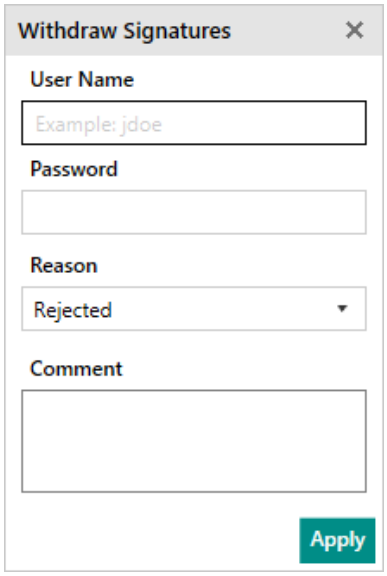
1 Go to "Operating Procedures" section.

2 Right click on the desired Operating Procedure and click on **[Withdraw all Signatures]**.



3 Enter Login and choose a reason for withdraw.

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



4 Click on **[Apply]**

"Unsigned" is now displayed in the "Signature" row of the object.

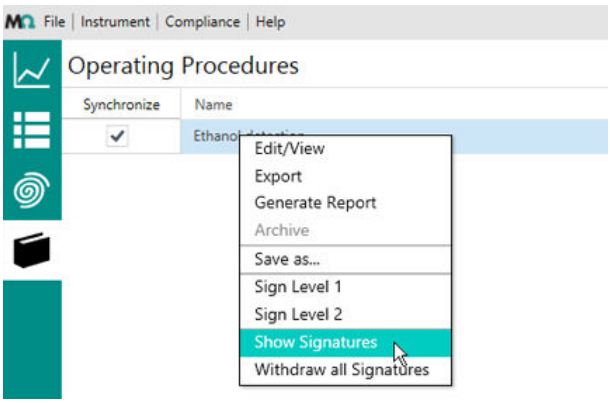
Show Signatures of operating procedures, training sets and libraries

NOTE

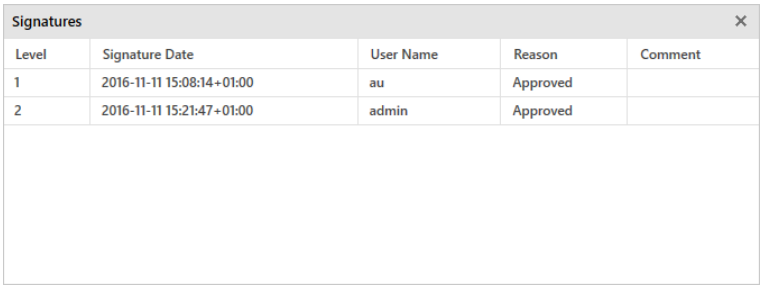
Show signatures of samples works different, refer to next procedure.

1 Go to "Operating Procedures" section.

2 Right click on the desired Operating Procedure and click on **[Show Signatures]**.



Available signatures are displayed.



Show Signatures of samples

1 Go to "Samples" section.

2 Right click on the desired Sample and click on **[Information]**.

3 Change to tab "Signatures".

Available signatures are displayed.

4.11.2 User management

General information

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

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

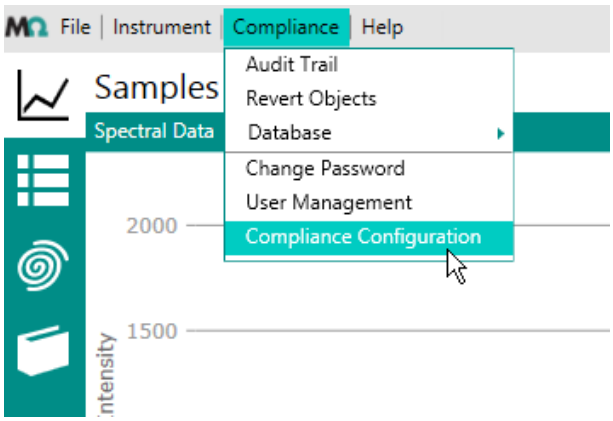
To be in compliance with FDA regulations, a user management must be configured. Security settings can be activated according to 21 CFR Part 11 by activating the relevant check boxes. The following conditions will then be complied with:

- 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).

4.11.3 Compliance configuration

NOTE

Only administrators have access to this area.



Compliance Configuration can be found in **Compliance ▸ Compliance Configuration**.

The following settings can be configured:

Option	Description
Minimum Password length	A minimum password length can be defined here.
Login attempts	How many login attempts with wrong password are allowed until the user will be disabled.
Special character required	If activated, every password must contain at least one special character. On the touch keyboard of the instrument, the amount of special characters is limited. Therefore not all existing special characters are supported. If a user chooses a new password, the software checks if an invalid special character is in. An error message will be displayed, that the password contains invalid character.
Password expires	

Option	Description
Automatic logoff	If the automatic logoff is activated, the user will automatically be logged off the Mira Cal software after the pre-defined time without any user interaction. If an instrument is connected, it will be disconnected.
Admin Only Archiving	If activated, only a user with admin rights is allowed to archive objects for example operating procedures.
Save Comment required	If a Save Comment is required, the user has to enter a comment at any time he changes an object. If, for example, the user changes a library, a dialog window opens before saving the changes. The user has to enter a comment before saving is possible.
Sync only signing Ops	If active, only operating signatures which are signed on Level 1 and Level 2 to can be synchronized with the instrument.
Force Device Calibration	If active, a calibration of the instrument must be performed after the defined period (in hours).

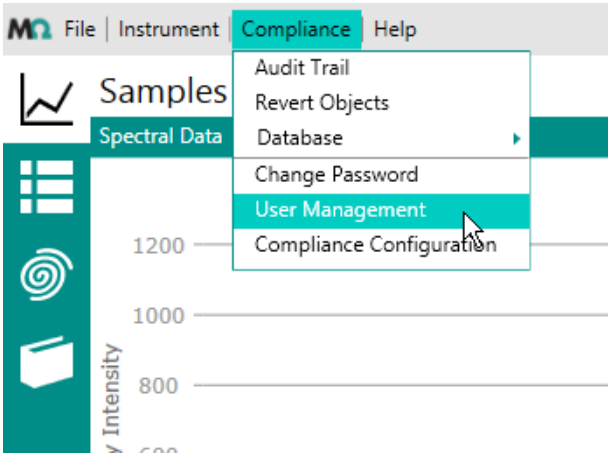
4.11.4 Manage users

NOTE

Only administrators have access to the user management area.

Create a user

1 Go to **Compliance** ▸ **User Management**



2 Click on **[Create user]**

3 Fill in all required information.

- User name:
  - Must not be empty.
  - Must be unique (Error if a user name already exists).
- Full name:
  - Must not be empty.
- Group:
  - **Routine User** Connect to 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: user management area, updates (firmware update, driver for instrument).
- Start password:
  - Minimum password length is pre-defined according to settings.
  - If activated in settings, at least one special character has to be used.
  - The user has to change the start password on first login.
- Confirm start password:
  - Must be equal to the field "Start password".

4 Click on **[OK]** to create the user.

5 The new user has to login to Mira Cal and change his start password.

NOTE

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

Reset 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 two times into the input fields. Click on **[Change]**.

NOTE

Last 5 of the expired passwords may not be reused.

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.

NOTE

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 software.

Change own password

1 Go to **Compliance ▸ Change Password**

2 Enter old password.

Enter new start password two times into the input fields. Click on **[OK]**.

NOTE

Last 5 of the expired passwords may not be reused.

The new password is active for the next Mira Cal login.

Disable/Enable users

1. Go to **Compliance ▸ User Management**
2. Select a user in the list and click on **[Edit User]**.
3. Below the input fields enable or disable the checkmark "Disable User".
4. Click on **[OK]**.

   Affected users will no more have access to Mira Cal software. At a login attempt a dialog window will appear to contact the administrator.

NOTE

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.

5 Malfunctions and troubleshooting

5.1 Create 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 Metrohm representative.

A calibration standard has to be connected.

1 Click on **Instrument ▸ Create Support File**.

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

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

6 Accessories

Up-to-date information on the scope of delivery and optional accessories for your product can be found on the Internet. You can download this information using the article number as follows:

Downloading the accessories list

1. Type *https://www.metrohm.com/* into your Internet browser.
2. Under **Find products, accessories, and applications by**, enter the article number (e.g. **2.1001.0010**).
3. Under **Products**, click on **More information**.

   Detailed information regarding the product is shown on various tabs.
4. On the **Included parts** tab, click on **Download the PDF**.

   The PDF file with the accessories data will be created.

NOTE

When you receive your new instrument, we recommend downloading the accessories list from the Internet, printing it out and keeping it for reference purposes.