

# Misa Cal



Tutorial

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# Misa Cal

1.1.0 or higher

**Tutorial**

8.0105.8024EN /  
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# 1 Overview

## 1.1 Misa Cal – Program description

Misa Cal software is used together with the Metrohm Instant SERS Analyzer (Misa). Misa Cal is connected to Misa via USB.

### Misa Cal

- Administration
  - Operating procedure building
  - Custom SERS library building
- View results
- Generate reports
- Share results and reports
- Store all data

### Misa

- Analyze samples

### Synchronization between Misa and Misa Cal

On connection with Misa, Misa Cal ensures that the instrument is up to date. All settings and data are stored on the software and not on the instrument.

## 1.2 Misa Cal – Product versions

The product is available in the following versions:

*Table 1 Product versions*

Order number	Designation	Version feature
6.607.1010	Misa Cal	1.1.0 or higher

To download the latest version of Misa Cal, click on the following link:

<https://www.metrohm.com/en/support-and-service/software-center/>



## 1.3 About the documentation



### NOTICE

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

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

#### Symbols and conventions

The following icons and formatting may appear in this documentation:

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

## 1.4 Additional information

#### Hardware manual

Refer to following hardware manual for more information about the instrument.

- Misa product manual (8.950.8001)

#### Misa Cal M tutorial

Refer to following tutorial for more information about the companion mobile app for Misa.

- Misa Cal M tutorial (8.0105.8025)



## 2 Safety

### 2.1 Product safety

This product exhibited no flaws in terms of technical safety at the time it left the factory. To preserve this status and ensure non-hazardous operation of the product, the following instructions must be observed carefully.

### 2.2 Hazard levels

The following warning messages indicate the severity of the danger and its possible effects.



#### **DANGER**

##### **Immediate danger of life**

Irreversible injuries that will result in death.

Warns of dangerous situations or unsafe actions that will most certainly cause severe injuries or death.

Lists measures to avoid hazard.



#### **WARNING**

##### **Severe health hazards**

Serious injuries that could result in death.

Warns of dangerous situations or unsafe actions that could result in serious injuries or death.

Lists measures to avoid hazard.



## CAUTION

### Health hazards or severe property damage

Warns of dangerous situations or unsafe actions that could result in moderate injuries or considerable property damage.

Lists measures to avoid hazard.

## 2.3 Warning symbols

Make sure that any additional hazard symbols are marked on the product for your operation of the product.

The following warning symbols in the documentation and at hazard areas of the product point out hazard potentials:



– Warning of a hazard area



## NOTICE

### Warning symbol on the product

If this warning symbol is on the product, read the respective documentation prior to installation and initial start-up.



– Warning of electric shock from electrical potential



– Warning of danger of fire and explosion from highly flammable substances and gases



– Warning of danger of poisoning and chemical burns from chemical hazardous substances



– Warning of danger of infection and poisoning from biological hazardous substances



– Warning of risk of injury from high temperatures



– Warning of cut injuries from pieces of broken glass and/or sharp edges



– Warning of risk of injury by laser radiation



– Warning of dangerous optical radiation

## 2.4 Intended use

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

Usage therefore requires the user to have basic knowledge and experience in handling chemicals. Knowledge with respect to the application of the fire prevention measures prescribed for laboratories is also mandatory. Be sure to take proper safety precautions when working with chemicals.

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

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

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

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

The EU declaration of conformity loses its validity if modifications are carried out on the instruments and/or the components.

## 2.5 Residual risks

### 2.5.1 General dangers at the workplace

Generally, the regulations and provisions of the regulatory institutions and authorities in the field of work apply.

The instructions regarding the following areas have to be followed when using the products:

- Work safety
- Handling mechanical installations
- Handling electricity
- Handling hazardous and environmentally damaging substances
- Handling hazardous and environmentally damaging liquids

- Disposing hazardous and environmentally damaging substances

If they are not followed, this may result in:

- Disturbing, injuring and/or killing of people
- Malfunction and/or damage to instruments and infrastructure
- Damage and/or contamination of the environment



## WARNING

### General dangers at workplace

If the safety measures are not followed, working in a laboratory bears a high risk of injury, which can endanger life and health.

- Only professionally trained and qualified specialist personnel may operate the products.
- Follow the applicable provisions concerning work safety and all regulations on wearing protective clothing.
- Use suitable tools to perform your work.
- Check the fill level of waste bottles or waste canisters and analysis vessels, and make sure they do not overflow.
- Use protective grounding when working with highly flammable substances and gases.

## 2.5.2 Danger from electrical potential



## WARNING

### Electric shock from electrical potential

Risk of injury by touching live components or through moisture on live parts.

- Never open the housing of the instrument.
- Protect live parts (e.g. power supply unit, power cord, connection sockets) against moisture.
- If you suspect that moisture has gotten into the instrument, disconnect the instrument from the energy supply. Then notify Metrohm Service.
- Only personnel who have been issued Metrohm qualification may perform service and repair work on electrical and electronic components.
- The electrical safety of the instrument is ensured as part of the international standard IEC 61010.

### 2.5.3 Laser safety



## WARNING

### Risk of injury by laser radiation

Misa is a class 1 laser product and is safe under all conditions of normal use. Use of controls or adjustments or performance of procedures other than those specified in the user manual may result in exposure to hazardous levels of laser radiation.

- Follow the safety measures and instructions.
- Do not use the instrument in a manner that is not specified in the user manual.
- Do not open the housing of the instrument.
- Do not disable or circumvent the interlock protection mechanism of the Smart Tips.
- 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.

### Laser classification depending on Smart Tips

Attached Smart Tip	Laser Class 1
Calibration Standard	<b>X</b>
Misa Vial Holder	<b>X</b>
P-SERS Attachment	<b>X</b>

Calibration Standard, Misa Vial Holder, and P-SERS Attachment have an interlock mechanism for measurement. This mechanism prevents laser radiation from emerging.

The laser stops immediately if:

- The lid of the Smart Tip is opened.
- The attached Smart Tip is disconnected from the instrument.

#### 2.5.4 Danger from radiofrequency radiation



### CAUTION

#### Exposure to radiofrequency radiation

This equipment complies with FCC radiation exposure limits set forth for an uncontrolled environment.

- This equipment should be installed and operated with a minimum distance of 20 cm between the radiator and your body.

## 2.6 Responsibility of the operator

- Eliminate defects or damage which impair operating safety without delay.
- Eliminate malfunctions which could impair safety without delay.
- The rules, regulations and instructions listed in the present document are not the only valid ones. Comply with the applicable statutory rules, government agency directives and regulations.
- Unauthorized modification of the products excludes any and all liability on the part of the manufacturer for any damage resulting from this as well as for any consequential damage. No modifications, attachments or conversions which could impair safety may be carried out on the products without the approval of the manufacturer.
- Spare parts must meet the technical requirements established by the manufacturer. Original spare parts always meet these requirements.
- Personnel must be familiar with this safety-relevant information and it must be available for consultation at all times.

## 2.7 Personnel requirement

Only qualified personnel may operate this product. A qualified person is a user who has thoroughly reviewed this document and has a comprehensive understanding of the operations of the instrument.

The instrument is used for the analysis of chemical compounds, some of which may be hazardous. The user must be capable of recognizing and avoiding possible dangers, and be aware of standards, laws and regulations governing the handling of such chemicals.

## 3 Functional description

### 3.1 Misa Cal – Overview

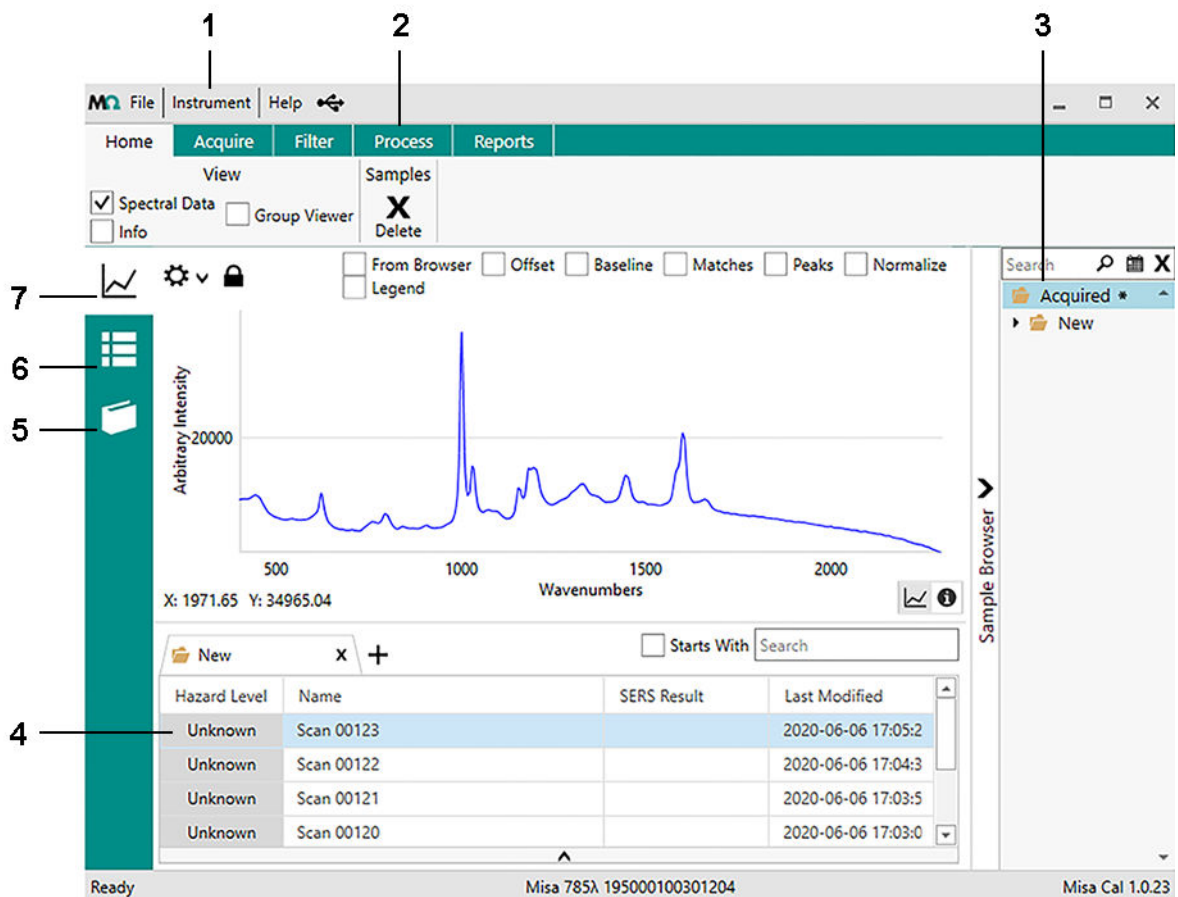


Figure 1 Misa Cal – General overview

**1 Selection menus**

**2 Function tabs**

**3 Sample browser**

**4 Sample list**

**5 Operating procedure view**

**6 Library view**

**7 Sample view**



### 3.2 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.

Users can build operating procedures by using parameters that the user selects in Misa Cal. Operating procedures can be shared between Misa Cal and Misa Cal M. Operating procedures created on Misa Cal and Misa Cal M can be used with any Misa instrument.

### 3.3 Selection menus


<b>File</b>	
<b>Open ▶</b>	
<b>Samples</b>	Imports samples.
<b>Libraries</b>	Imports libraries.
<b>Operating Procedures</b>	Imports operating procedures.
<b>Save As ▶</b>	
<b>Samples</b>	Saves samples to selected location.
<b>Libraries</b>	Saves libraries to selected location.
<b>Operating Procedures</b>	Saves operating procedures to selected location.
<b>Settings</b>	Opens a view with two tabs: <ul style="list-style-type: none"> <li>▪ General (see "General tab", page 12)</li> <li>▪ Reports (see "Reports tab", page 14)</li> </ul>
<b>Advanced ▶</b>	
<b>Database</b>	<ul style="list-style-type: none"> <li>▪ <b>Info</b> Lists database information.</li> <li>▪ <b>Back Up</b> Backs up the database.</li> <li>▪ <b>Restore</b> Restores the database.</li> <li>▪ <b>Set Location</b> Sets the location of the database.</li> </ul>



<b>Change Language</b>	<ul style="list-style-type: none"> <li>▪ <b>Import Licensed Libraries</b> Imports licensed libraries.</li> <li>▪ <b>Import Mobile App Database</b> Imports the database from Misa Cal M.</li> <li>▪ <b>Reset</b> Removes all items from the database, including operating procedures, samples and libraries.</li> </ul>
<b>Service Portal</b>	Changes the language of the application.
<b>Exit</b>	Allows access for service engineer. Closes Misa Cal.

<b>Instrument</b>	
<b>Connect</b>	Connects Misa to Misa Cal.
<b>Disconnect</b>	Disconnects Misa from Misa Cal.
<b>Enable Misa One Touch</b>	Only available if Misa One Touch mode is disabled. Click to enable Misa One Touch mode.
<b>Disable Misa One Touch</b>	Only available if Misa One Touch mode is enabled. Click to disable Misa One Touch mode.
<b>Set Remote Acquire OP</b>	Displays only if Misa One Touch mode is enabled. Click to define the operating procedure to be used with Misa One Touch mode. The default is the <b>ID Kit OP</b> . An OP must be saved in Misa Cal before it can be selected for use in Misa One Touch Mode.
<b>Bluetooth PIN code</b>	Displays only when Misa is connected to Misa Cal. Change the PIN code for the Bluetooth® connection with Misa Cal M. The default PIN code is 9999.
<b>System Suitability Test Archive</b>	Lists all system suitability tests in the database.
<b>Info</b>	Lists identification information of Misa and the operating system.
<b>Rename</b>	Displays only if Misa is connected to Misa Cal. Change the name of Misa if necessary.
<b>Execute Script</b>	Execute service scripts for minor adjustments to Misa.



<p><b>Calibrate Instrument</b></p> <p><b>System Suitability Test</b></p> <p><b>Updates ►</b></p> <p><b>Import Certificate Package</b></p>	<p>Follow the prompts.</p> <p>The system suitability test can be run immediately following calibration.</p> <p>Runs the system suitability test independently of calibration routine.</p> <p>Follow the prompts.</p> <p>Updates licensed libraries.</p>
<p><b>Help</b></p> <p><b>About</b></p> <p><b>Create Support File</b></p>	<p>Displays Misa Cal version and copyright.</p> <p>Generates a support file for the desktop software and Misa.</p> <p>Select <b>[Okay]</b> when asked to attach the Calibration Standard.</p> <p>A support file is generated.</p> <p>The support file can be saved or sent to Metrohm Raman should there be issues with the device or desktop software.</p>
<p><b>Connected</b> </p>	<p>Displays when Misa is connected to Misa Cal.</p>

**General tab**

**File ► Settings**

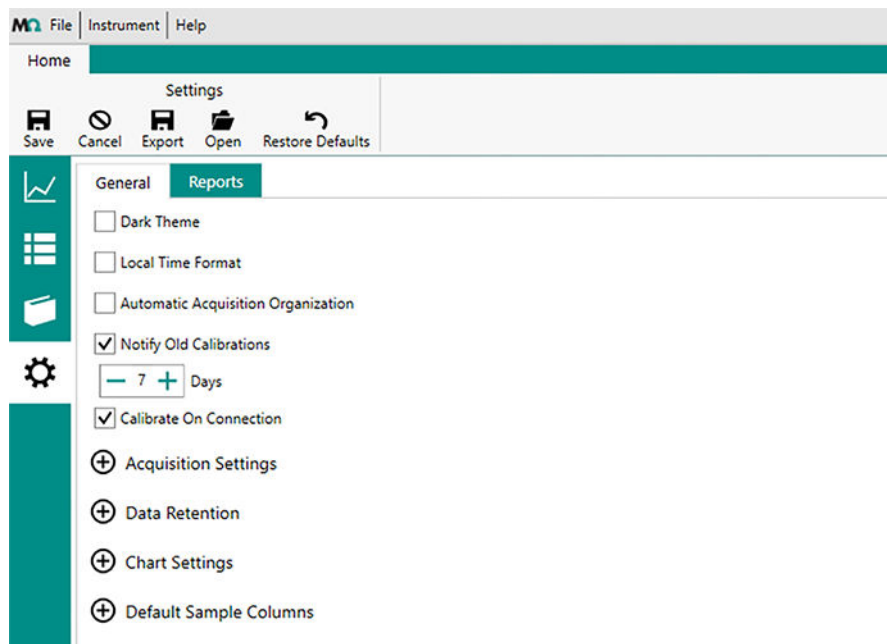


Figure 2 Settings - General tab

In the General tab you can set the following:

General tab	
<b>Dark Theme</b>	Sets the software background to the color black.
<b>Local Time Format</b>	Sets the time to the local computer format.
<b>Automatic Acquisition Organization</b>	Automatically creates a folder with the serial number of Misa. Additionally, saves the time and date of acquisitions performed by Misa Cal.
<b>Notify Old Calibrations</b>	Gives a pop up reminder if the time since the last calibration is longer than the set time period.
<b>Calibrate On Connection</b>	Prompts the user to calibrate Misa on first connection.
<b>Acquisition Settings ▶</b>	
<b>Show Results Popup on Remote Sample Received ▶</b>	Display results on sample acquisition.
<b>Standard Match Generic Acquisitions</b>	Sets parameters for matching.



<b>SERS Matching Generic Acquisitions</b>	If activated, the SERS matching algorithm is used.
<b>Data Retention ▶</b>	
<b>Retain All Data</b>	Retains all data in the database. If deactivated, the time period of expiration of the data, the data clearing frequency and settings for the database backup can be chosen.
<b>Chart Settings ▶</b>	
<b>Y Grid Lines</b>	Displays Y grid lines in the sample chart.
<b>X Grid Lines</b>	Displays X grid lines in the sample chart.
<b>Invert X Axis</b>	Inverts X axis in the sample chart.
<b>Chart Line Thickness</b>	Defines chart line thickness.
<b>Default Sample Columns</b>	Defines the sample columns displayed in the <b>Sample</b> view.

### Reports tab

#### File ▶ Settings

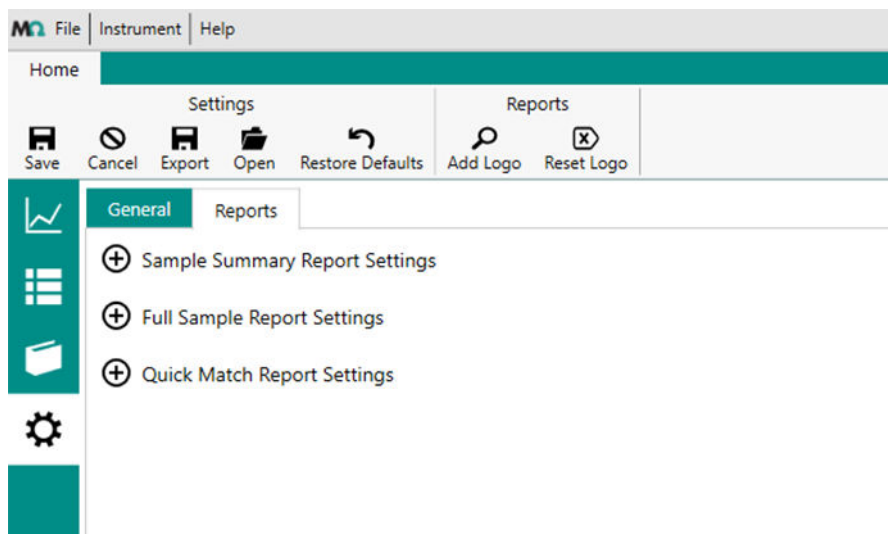




Figure 3 Settings - Reports tab

In the Reports tab you can set the following:

#### Reports tab

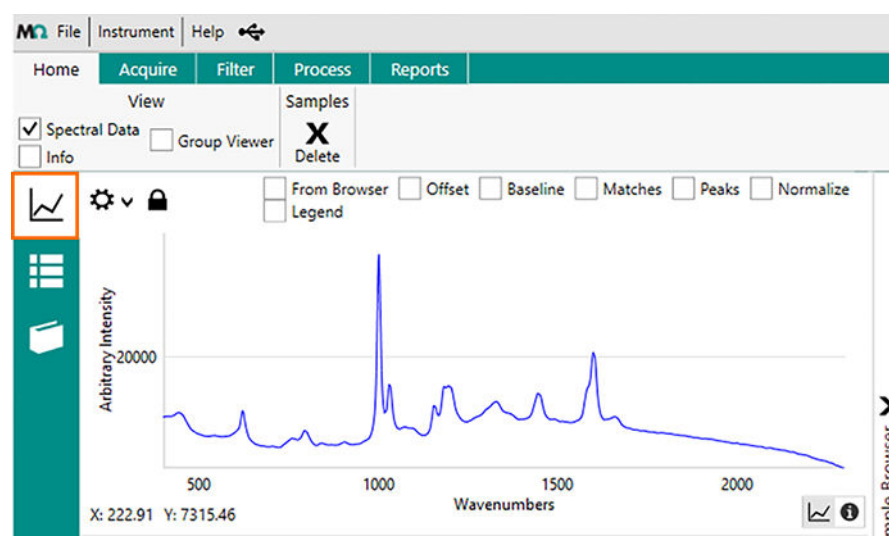
<p><b>Sample Summary Report Settings</b></p>	<p>The selected settings define the content of the <b>Sample Summary</b> report.</p> <p>Click on  <b>View Example</b> to view, save or print the report.</p> <p>To add a personalized logo to the report, click on <b>Add Logo</b> in the <b>Reports</b> section of the <b>Home</b> tab.</p>
<p><b>Full Sample Report Settings</b></p>	<p>The selected settings define the content of the <b>Full Sample</b> report.</p> <p>Click on  <b>View Example</b> to view, save or print the report.</p> <p>To add a personalized logo to the report, click on <b>Add Logo</b> in the <b>Reports</b> section of the <b>Home</b> tab.</p>
<p><b>Quick Match Report Settings</b></p>	<p>The selected settings define the display of the <b>Quick Match</b> report.</p>


### 3.4 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
- **Operating Procedure** view

#### Sample view

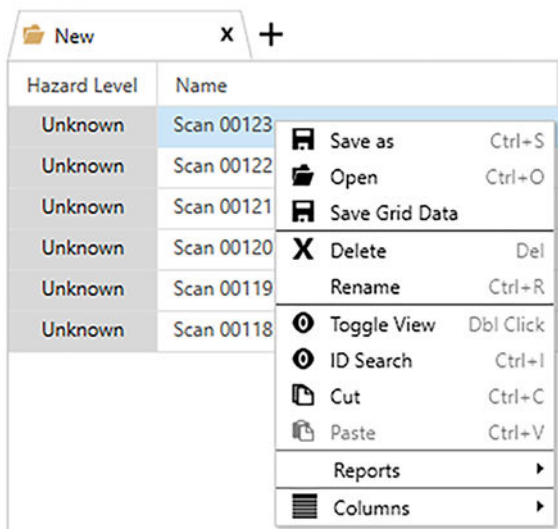


<p><b>Sample</b> </p>
<p>Home ►</p>
<p>Samples</p>

Click on a sample in the sample list to highlight and carry out actions.



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



**Acquire** ►

This is displayed only when Misa is connected to Misa Cal.

**Acquisition Settings**

Select the acquisition settings for scanning a sample while Misa is connected to Misa Cal. See *"Acquiring data with Misa"*, page 38.

**Filter**

Select parameters to sort samples.

**Process**

Select a sample and reprocess the data against different libraries.

- **Identification**

Perform a Pearson's correlation match against the chosen library.

- **SERS Identification**

Perform matching against the chosen SERS library.

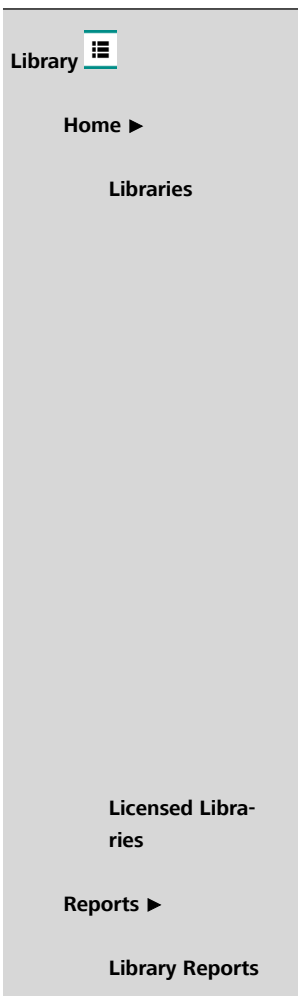
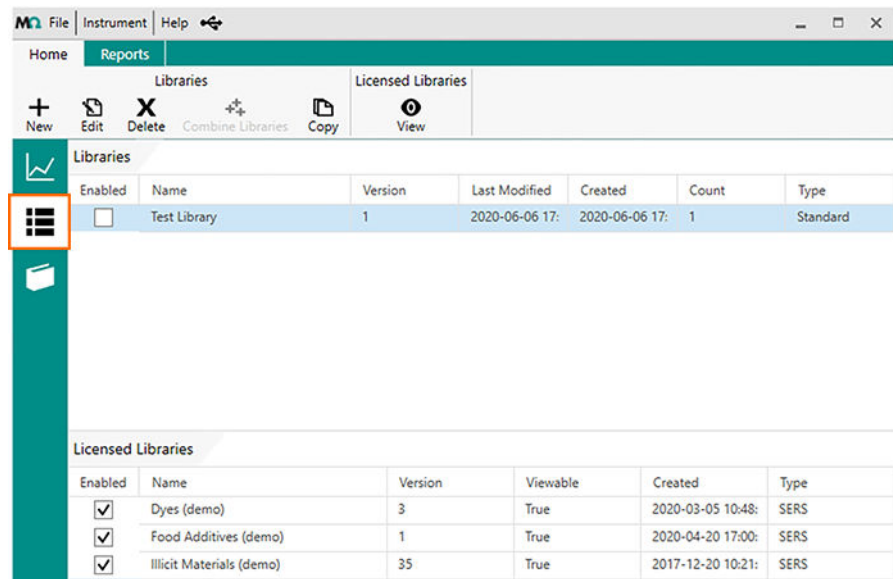
- **Spectral Math**

Add or subtract two spectra or perform other mathematical operations on selected data.

**Reports**

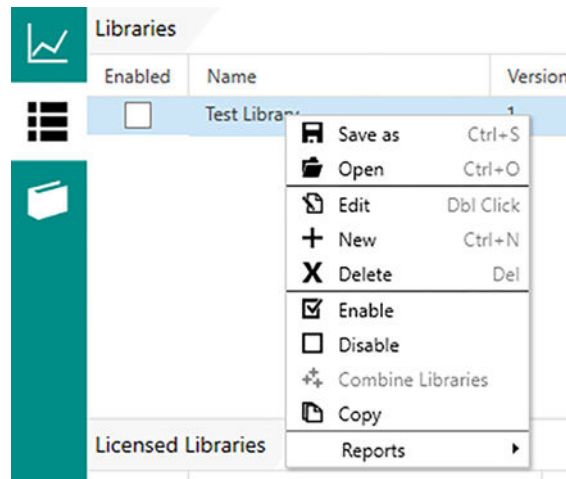
Generate reports for the selected spectra.

## Library view



Click on a library to highlight and carry out actions.

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

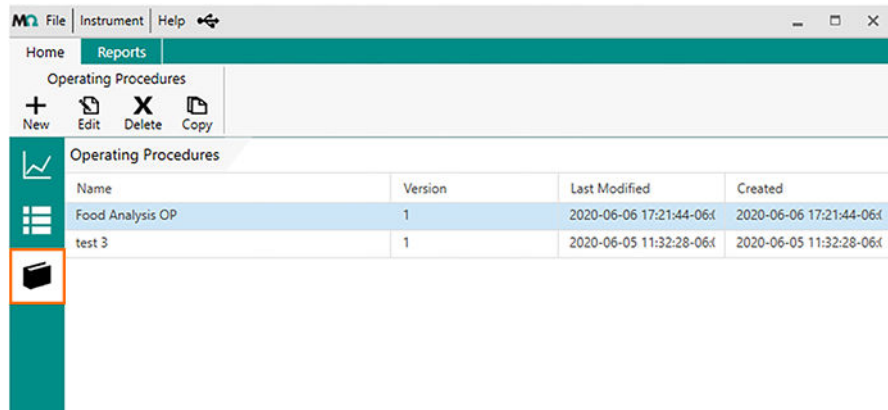


Select a licensed library and click on **View**.

Generate reports for the selected libraries.



### Operating procedure view



**Operating Procedures**

Home ►

**Operating Procedures**

**Reports**

Click on an operating procedure to highlight and carry out actions.  
 No actions can be taken on the default OP.  
 Right click on a selected operating procedure to open a function menu.

Generate a report for the selected operating procedures.



## 3.5 Identifying samples with libraries

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

**SERS Demo Libraries**, created by Metrohm Raman, are preinstalled on Misa. Libraries can also be created by the user or purchased from Metrohm.

### Creating a library

Users can create a library in Misa Cal, which will then be used for identification of samples. Identification libraries are generated in Misa Cal from acquisitions of known substances that the user has access to.

### 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.

2 types of matching are available on Misa Cal:

1. **HQI**: 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, **No Results** will be displayed.
2. **SERS algorithm**: The measured sample will be compared to the libraries by peak location and any results are identified as **SERS Identification Result**. If there is no match of the sample to a library, **No Results** will be displayed.

For more information about processing data and types of matching available on Misa Cal see "*Processing a spectrum*", page 40.

## 4 Installation

### 4.1 System requirements



#### NOTICE

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

<i>Processor</i>	Multicore x86 processor (64-bit preferred)
<i>Operating system</i>	<ul style="list-style-type: none"> <li>▪ Windows 10 (64-bit only)</li> <li>▪ Windows 7 (Service Pack 3 or higher). In January 2020, Microsoft will discontinue support for Windows 7. Support for Metrohm Raman software will end with the Microsoft lifecycle.</li> </ul>
<i>Screen resolution</i>	Resolution 1024 x 768 or higher
<i>RAM</i>	All operating systems: 2 GB minimum; 4 GB recommended
<i>Storage capacity</i>	Minimum 100 GB; 500 GB recommended
<i>USB connectors</i>	USB 2.0, external powered USB 2.0 hub recommended
<i>Mouse and keyboard</i>	Required, USB, PS/2 style, or wireless
<i>Keyboard</i>	Compatible keyboard using USB / PS/2, or similar connection
<i>System backup</i>	Network or local backup required for data archiving.

### 4.2 Installing Misa Cal

#### Prerequisite:

For the installation of Misa Cal administrator rights are required.

Make sure the system fulfills the system requirements. See "System requirements", page 20.

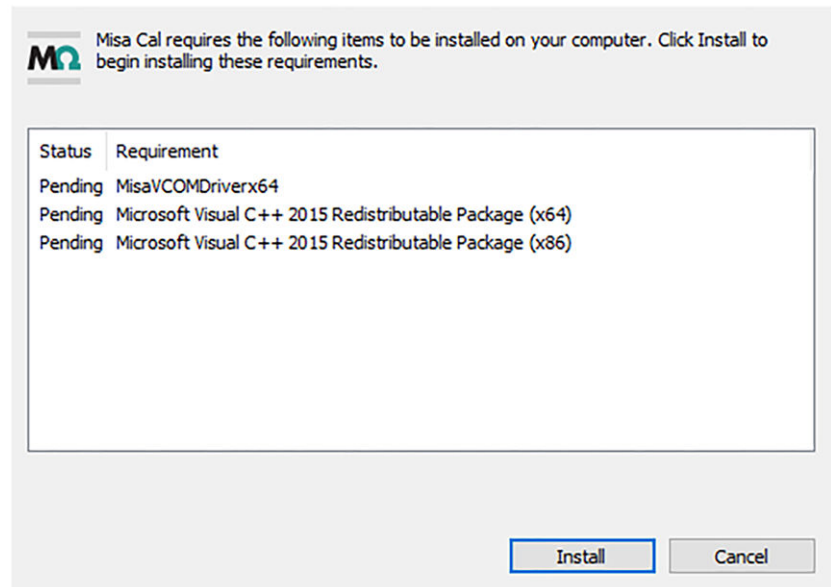
- 1 To download the latest version of Misa Cal, click on the following link:

<https://www.metrohm.com/en/support-and-service/software-center/>

Double click on the installer.

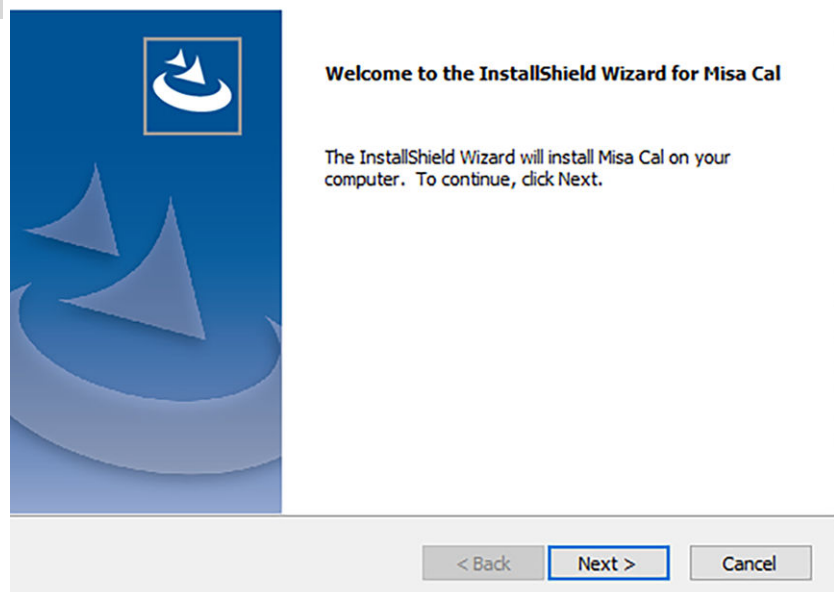
2 Click on **[Yes]** in the appearing window and follow the wizard on the screen.

3 Misa Cal - InstallShield Wizard

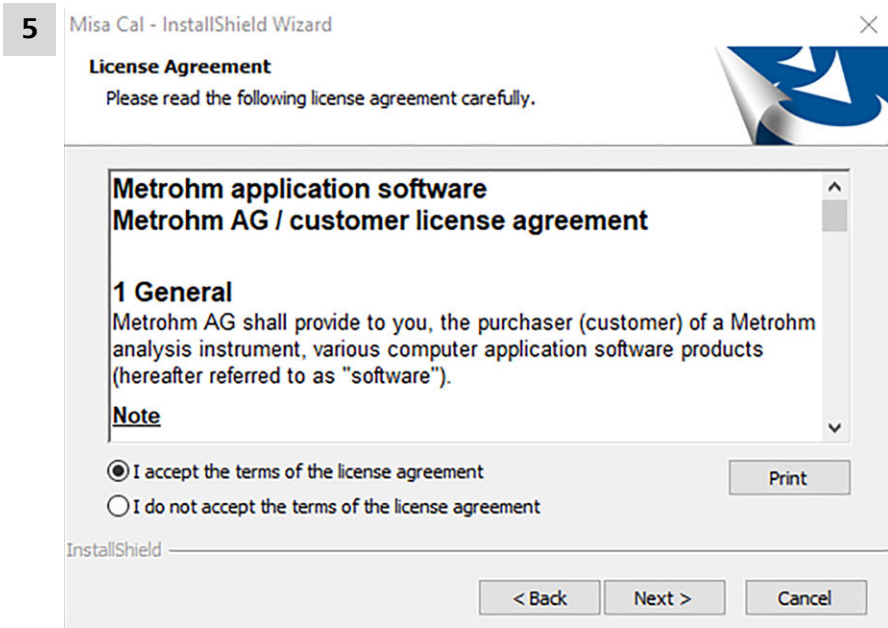


Click on **[Install]**.

4 Misa Cal - InstallShield Wizard

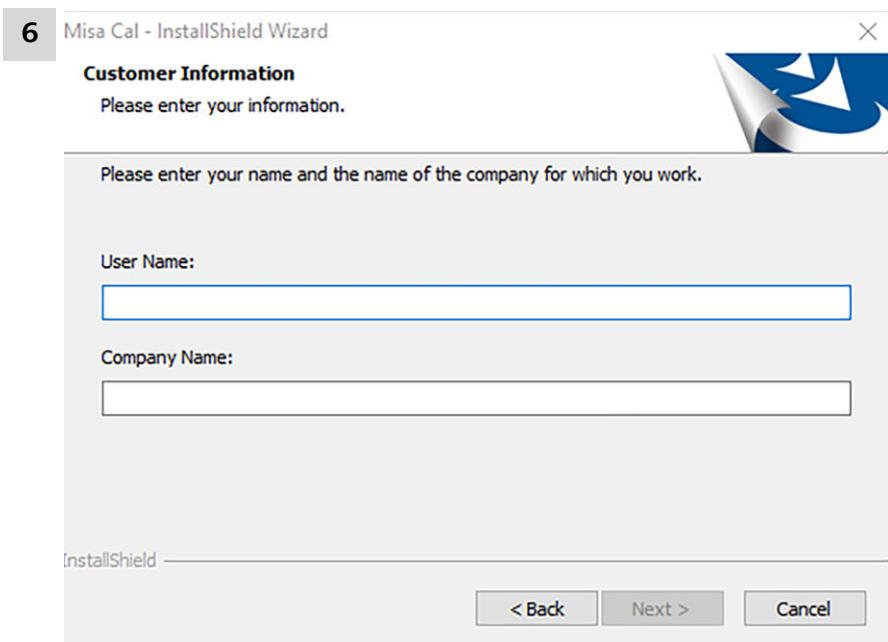


Click on **[Next]** to start the installation of Misa Cal.



Select **I accept the terms of the license agreement**.

Click on **[Next]**.



Enter your **User Name**.

Enter the **Company Name**.

Click on **[Next]**.

**7** Misa Cal - InstallShield Wizard**Select Features**

Select the features setup will install.

Select the features you want to install, and deselect the features you do not want to install.

Feature	Size
<input checked="" type="checkbox"/> Misa Cal	537 MB

Description  
Misa Cal Installation

Change...

Space Required on C: 537 MB  
Space Available on C: 262892 MB

InstallShield

< Back Next > Cancel

Select Misa Cal and click on **[Next]**.

**8** Misa Cal - InstallShield Wizard**Ready to Install the Program**

The wizard is ready to begin installation.

Click Install to begin the installation.

If you want to review or change any of your installation settings, click Back. Click Cancel to exit the wizard.

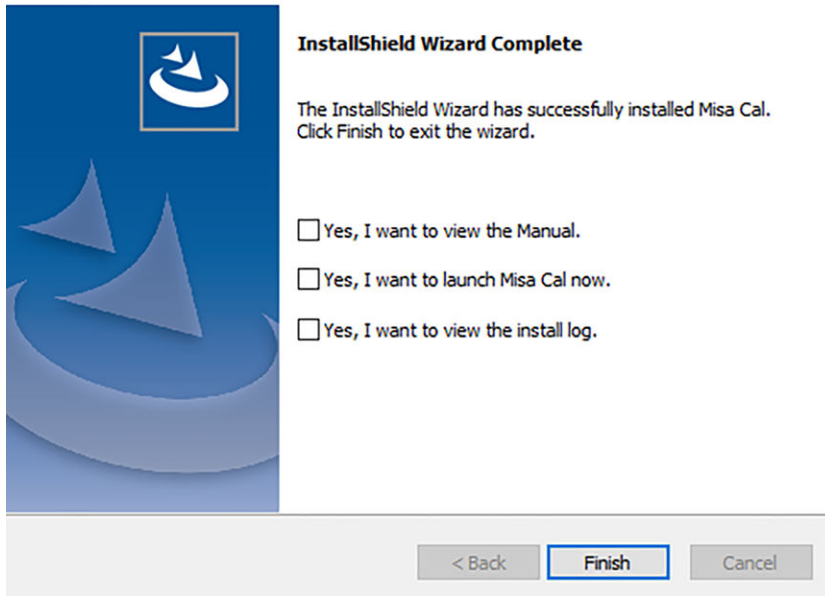
InstallShield

< Back Install Cancel

Click on **[Install]** to start the installation.



9 Misa Cal - InstallShield Wizard



Click on **[Finish]** to complete the installation.



## 5 Initial start-up

Misa Cal is designed to operate as simply as possible. The main use of Misa Cal is to control Misa for data acquisition and report generation. This is accomplished by simply connecting Misa to Misa Cal. Acquired data will automatically synchronize, results and reports will be generated. A sample summary report is the default, but full report generation can be set as the default in the software setting tab. Advanced features include custom operating procedure creation and library building.

### 5.1 Connecting Misa to Misa Cal via USB

#### Prerequisite:

- Misa is switched on.
- 

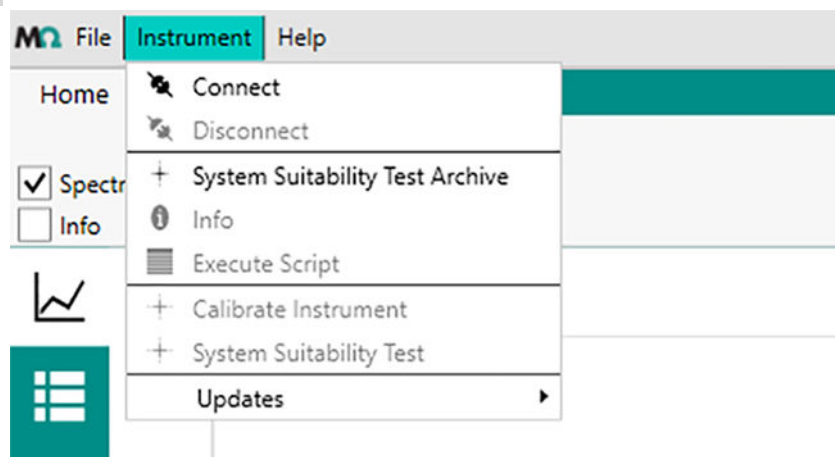
#### 1 NOTICE

Only use the provided Metrohm USB Mini-B cable (6.2151.110).

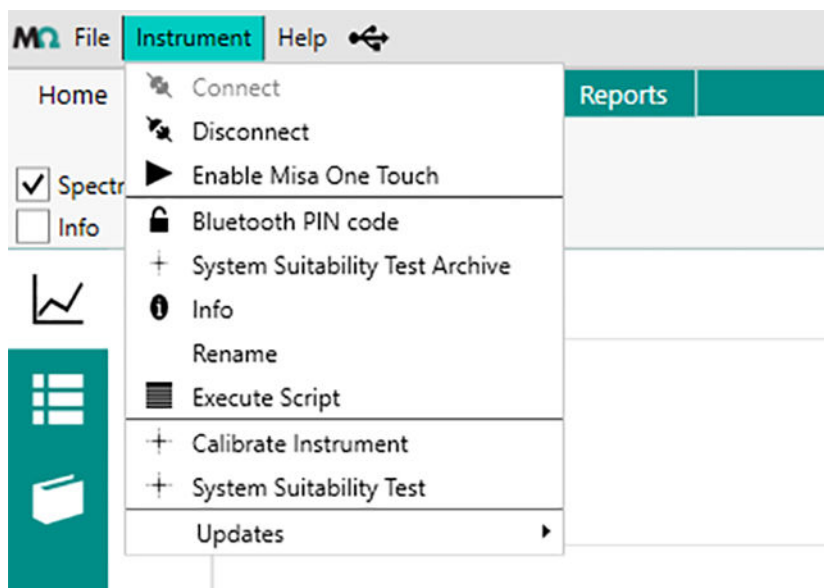
Connect Misa to the computer using the USB Mini-B cable.

2 Double click on the Misa Cal desktop icon to start the software.

3 To connect Misa to Misa Cal, click on **Instrument ► Connect**.



4 To disconnect Misa from Misa Cal, click on **Instrument ► Disconnect**.



## 5.2 Configuration

### 5.2.1 Creating and editing libraries

Spectra for user-created 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).



#### NOTICE

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

- 5 Activate the library Type **[Standard]** or **[SERS]**.





## NOTICE

The library type defines the type of matching that can be performed. SERS libraries can only be matched by comparison of peak locations. Standard libraries can only be matched by Hit Quality Index (HQI). A library must be either of Standard type or SERS type. See *"Processing a spectrum"*, page 40.

### 6 Adding samples

Go to the **Add Samples** tab.

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



## NOTICE

Use the **Sample Browser** to find samples. Go to the **Recent** tab to view recently viewed samples.

- 8 Double click on the sample or click on **[Add]** in the **Library Samples** section of the **Home** tab to add the sample to the library.

- 9 Go to the **Library Samples** tab.

### 10 Adding metadata

Double click on the library sample in the sample list.

It will toggle to a **Library Sample Metadata** tab.

You can add the following information in this tab.

- Name
- CAS
- Hazard Level
- Sample Type
- Hazard Comment
- Synonyms
- GHS Classifications

This information is displayed in the Misa Cal identification screens.



## 11 Defining peaks for SERS library types

For SERS library types, the user must also define peaks that characterize the spectrum for matching. There are 2 options:

- 1. Activate **[Info]** in the **Home** tab.  
The tool for **SERS Regions** on the right hand side of the software window is displayed.
  - Enter the SERS regions, i.e. the left limit and right limit that defines a peak for the spectrum.  
Note that there must be at least one SERS region defined.  
Generally, the more peaks are defined for a spectrum, the likelihood of false positives is reduced.
  - Enter a noise region by choosing a region of the spectrum that does not contain any peaks.  
If possible, specify a noise level to improve matching. For SERS spectra, a noise region of  $1900 - 1950 \text{ cm}^{-1}$  is recommended.
  
- 2. Activate **[Spectral Data]** in the **Home** tab.
  - Enter the SERS regions by clicking **[Add]**.  
A pair of vertical lines appears over the spectrum.
  - Drag the pair of vertical lines over the desired peak to specify a peak location.  
Note that there must be at least one SERS region defined.  
Generally, the more peaks are defined for a spectrum, the likelihood of false positives is reduced.  
The tool for **SERS Regions** is displayed on the **Home** tab.
  - Enter the noise regions by clicking **[Add Noise Region]**.  
Another pair of vertical lines appears over the spectrum.
  - Drag the pair of vertical lines over a region of the spectrum that does not contain any peaks to specify the noise for the spectrum.  
If possible, specify a noise level to improve matching. For SERS spectra, a noise region of  $1900 - 1950 \text{ cm}^{-1}$  is recommended.

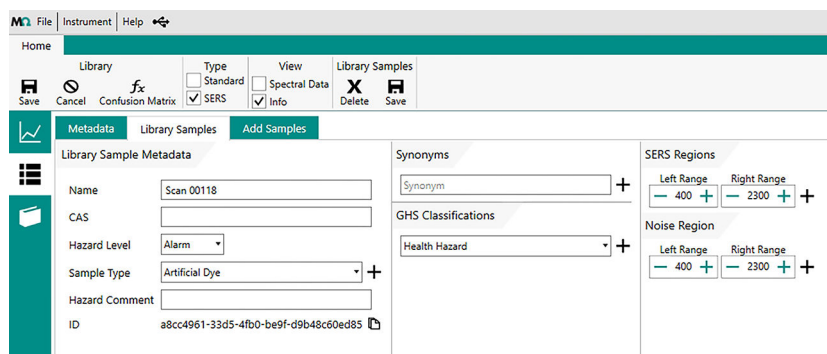


Figure 4 SERS regions (with Info checked)

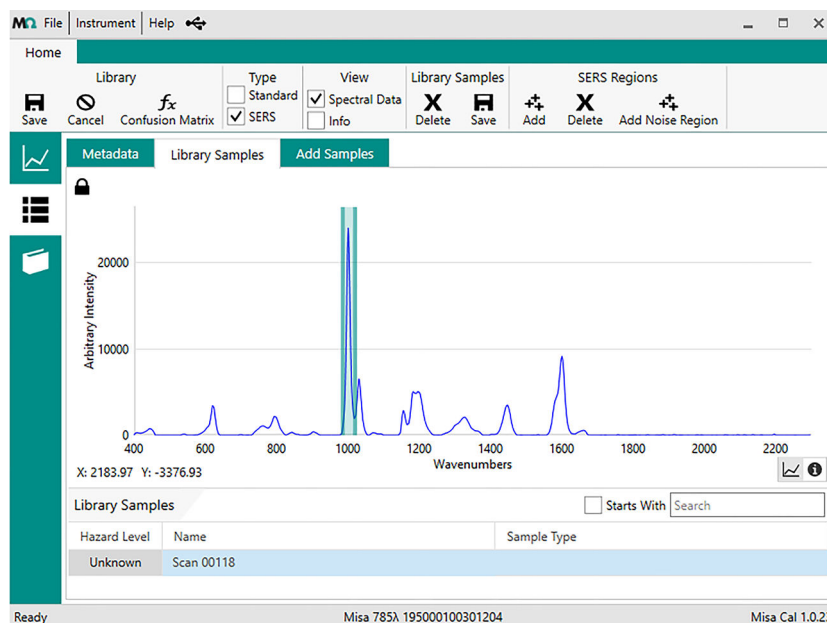


Figure 5 SERS regions (with Spectral Data checked)

- 12 Click on **[Save]** in the **Library Samples** tab to save sample meta-data.
- 13 Click on **[Save]** in the **Library** tab to create the new library.

### Editing an existing library

- 1 Go to the **Library** view.
- 2 Select a library and click on **[Edit]**.
- 3 The following options are available:
  - To add a sample, go to the **Add Samples** tab and select a sample.



- To add the sample to the library, double click on the sample or click on **[Add]** in the Library Samples section of the **Home** tab.
- To delete a sample, select a sample and click on **[Delete]** in the **Library Samples** section of the **Home** tab.

**4** Click on **[Save]**.

**5** Edit library sample metadata in the preexisting user libraries.



## NOTICE

Licensed libraries cannot be edited, they can only be viewed.

### 5.2.2 Creating and editing operating procedures

Operating procedures direct the acquisitions and evaluations of spectra. Users can create and save operating procedures that specifically define the following acquisition options.

- Selected laser powers
- Averaging
- Integration time
- Evaluation Processes

By creating operating procedures, users can avoid having to manually set parameters each time prior to performing an acquisition.

The following table shows all acquisition options for operating procedures.

*Table 2 Acquisition options*

Acquisition option	Description
<b>Operating Procedure Type</b>	<p>Operating procedures can be STANDARD or SERS type.</p> <p>Data collected with the STANDARD type can only be matched to STANDARD libraries using HQI. Data collected with the SERS type can only be matched to SERS libraries by peak comparison.</p>


Acquisition option	Description
<b>Smart Acquire</b>	<p>Laser power, integration time etc. are automatically adjusted to the type of sample, environment and amount of background lighting. This option is useful if acquisition settings cannot be defined.</p> <p><b>Smart Acquire</b> can only be used with STAND-ARD operating procedures.</p>
<b>Laser Power</b> (level)	<p>The intensity of the laser can be reduced. Choose a value between 1-5. 5 is the maximum.</p> <p>The recommended value is 5.</p> <p>Reasons to lower the laser power are:</p> <ul style="list-style-type: none"> <li>▪ Measuring critical samples that can vaporize easily.</li> <li>▪ Measuring materials with a low melting point. Liquid and solid forms of a compound have different spectra.</li> <li>▪ Avoid burning of SERS materials.</li> </ul>
<b>Auto Integration</b>	<p>The instrument automatically chooses the best Integration time for the current sample.</p>
<b>Integration Time</b> (sec.)	<p>The integration time indicates how long a single spectrum is recorded.</p> <p>The integration time is divided into two steps:</p> <ul style="list-style-type: none"> <li>▪ Laser <b>ON</b> to acquire sample spectrum.</li> <li>▪ Laser <b>OFF</b> to acquire reference.</li> </ul> <p>The actual time for a measurement is twice the entered value.</p> <p>The maximum integration time is 30 seconds.</p>
<b>Averages</b>	<p>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.</p> <p>The maximum number of averages is 30.</p> <p>Example: Enter <b>5</b> to have an averaged spectrum of 5 measured samples.</p>
<b>Smart Tip</b>	<p>Select the required attachment to measure your samples. If no dedicated smart tip is required, select <b>Allow all</b>.</p>



Acquisition option	Description
<b>Raster</b>	By default, Raster is on – i.e. laser is constantly moving over the sample during measurement. If unchecked, Raster is disabled, and laser is fixed on a spot in the sample.

**Creating a STANDARD operating procedure**


- 1 Go to the **Operating Procedure** view.
- 2 Go to the **Home** tab.
- 3 Click on **[New]**.
- 4 Select **[Standard]** type.
- 5 Add information about the operating procedure in the **Metadata** tab.



### NOTICE

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

- 6 Go to the **Acquisition** tab. Select the desired acquisition options.
- 7 Go to the **Identification** tab. Select the library to be used for matching from the **Available Libraries**.



### NOTICE

The library selected in a Standard type operating procedure must be a Standard library.

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

- 8 Double click on the library or click on **[Add]** in the **Identification** section of the **Home** tab to move the library to **Identification Libraries**.

To remove a library from **Identification**, select it and click on **[Remove]**.

- Select the minimum Hit Quality Index (HQI). The default value is 0.85.
- Activate **Enabled** to match against all user enabled libraries.
- Activate a targeted sub-library instead of searching the entire large library.

- 9 Click on **[Save]** in the **Operating Procedure** section of the **Home** tab to save the operating procedure.

The newly created operating procedure will be listed in the **Operating Procedure** view in the **Home** tab.

### Creating a SERS operating procedure

- 1 Go to the **Operating Procedure** view.
- 2 Go to the **Home** tab.
- 3 Click on **[New]**.
- 4 Select **[SERS]** type.
- 5 Add information about the operating procedure in the **Metadata** tab.



#### NOTICE

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

- 6 Go to the **Acquisition** tab. Select the desired acquisition options.
- 7 Go to the **SERS Identification** tab. Select the library to be used for matching from the **Available Libraries**.

To remove a library from **SERS Identification**, select it and click on **[Remove]**.

- Activate **Enabled** to match against all user enabled libraries on the instrument.
- Activate a targeted sub-library instead of searching the entire large library.



## NOTICE

The library selected in a SERS type operating procedure must be a SERS library.

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

**8** Double click on the library or click on **[Add]** in the **SERS Identification** section of the **Home** tab to move the library to **SERS Libraries**.

**9** Click on **[Save]** in the **Operating Procedure** section of the **Home** tab 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.

### Editing an existing operating procedure

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

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

**3** You can edit the following settings.

- **Type (Standard or SERS)**
- **Metadata**
- **Acquisition parameters**
- **Identification / SERS Identification**
- **Libraries** to match against

**4** Click on **[Save]**.



## 5.3 Calibration and system suitability

### Calibrating Misa

A calibration is performed to determine if acquisitions are within an acceptable range of parameters. To apply corrections use the Calibration Standard (6.07501.010). The Calibration Standard contains an ASTM 1840 reference sample for calibration. Calibration is recommended daily and additionally in the following situations:

- on receiving a new instrument,
- after a long period of non-usage,
- after service,
- after extreme environmental changes (e.g. a large change in temperature),
- mechanical shock (e.g. a drop).

**1** Connect Misa to Misa Cal.

**2** Attach the Calibration Standard to Misa.

**3** Ensure the instrument is sitting flat on its base to avoid calibration errors.

**4** Click on **Instrument ► Calibrate instrument**. The calibration may take some time.

A dialog confirms the success or failure of the calibration.

There will be a prompt to do a system suitability test.

**5** Select **[OK]** to automatically run the test. Or select **[Cancel]** to 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 can 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 Misa to Misa Cal.



**2** Attach the Calibration Standard to Misa.

**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. See "*Creating support log file*", page 50.

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

## 6 Operation and control

### 6.1 Smart Tips – Overview

Each Smart Tip allows an individual way of data acquisition. Smart Tips are attached to the instrument with magnetic connectors. Smart Tips contain a memory chip so that the instrument can identify them. Due to design, Smart Tips will not allow operation of Misa when seated in an incorrect position.

The following Smart Tips are available:

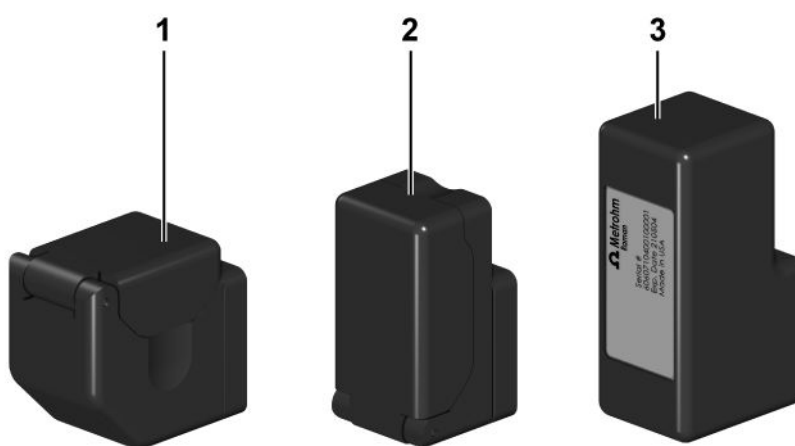


Figure 6 Misa – Smart Tips

#### 1 Misa Vial Holder (6.07505.040)

The Misa Vial Holder is used for samples in glass vials.

The interlock mechanism allows measurement with class 1 laser operation. The laser stops if the lid is opened.

#### 2 P-SERS Attachment (6.07505.030)

The P-SERS Attachment accommodates proprietary P-SERS substrates.

The interlock mechanism allows measurement with class 1 laser operation. The laser stops if the lid is opened.

#### 3 Calibration Standard (6.07501.010)

The Calibration Standard is needed for the calibration of the instrument. The Calibration Standard contains an ASTM 1840 reference sample.

## 6.2 Acquiring data with Misa

### Acquiring data with Misa connected to Misa Cal

#### Prerequisite:

Misa is connected to Misa Cal.

- 1 Click on the **Acquire** tab.
- 2 Select parameters.
  - Acquisition
    - **Single Acquisition**: Do not activate any boxes.
    - **Continuous Acquisition**: If activated, Misa executes scans until **[Stop Acquisition]** on the acquisition screen is clicked on.
    - **Multi Acquisition**: If activated, Misa executes a defined number of scans.  
Select the time interval between the sequential scans.
  - Acquisition settings
    - If the **Operating Procedure Acquire** box is deactivated, the **Acquisition Settings** tab appears.
    - If no boxes are activated, select **[Integration Time]**, **[Laser Power]** and the **[Number of Averages]**.
    - If **[Auto Integration]** is activated, the process determines the integration time. Select the laser power and the number of averages.
  - Operating procedure
    - Select operating procedures that are created in the software.
- 3 Click on **[Acquire]**.

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

### Acquiring data with Misa One Touch

Misa One Touch is a unique feature of Misa that allows acquisition of data by pushing the acquisition button on the instrument. Follow the steps below to activate Misa One Touch.

#### Prerequisite:

Misa is connected to Misa Cal.

- 1 In the Instruments tab, click on **[Enable Misa One Touch]**.

2



## NOTICE

An operating procedure must be saved in Misa Cal in order to be selectable for use with Misa One Touch.

Click on **[Set Remote Acquire Op]** to select the operating procedure to be used with Misa One Touch.

The default is the **ID Kit Op**.

3



## NOTICE

In Misa One Touch mode, it is not possible to perform continuous acquisitions or multiple acquisitions. Each time the acquisition button is pressed, Misa performs a single acquisition.

Push the acquisition button on the instrument to initiate an acquisition.

Spectra will be downloaded and displayed in the **Sample** view on completion of acquisition.

## 6.3 Displaying and managing data

### 6.3.1 Viewing a spectrum

When a spectrum is synchronized (i.e. the data is downloaded from the instrument onto the software), it is displayed in the **Samples** view. Double click on the spectrum name to view the matching results and the reference spectrum.

#### Setting a filter


- 1 Click on the **Filter** tab.
- 2 Set the desired filter criteria to display the corresponding spectra.
- 3 Click on **[Clear Filters]** to set the filters to default.

#### Displaying metadata

- 1 Double click on the chart to view the match results.

- 2 Click on the **Info** tab.  
The metadata is displayed.

### Adjusting the chart

- 1 Double click on the chart to view the match results.
- 2 Click on  to open the **Chart Settings**.
- 3 Select the desired viewing options.

### 6.3.2 Managing sample list folders

- 1 Go to the **Sample** view.
- 2 To create a folder, right click in the **Sample Browser** section and select **[New Folder]**.
- 3 Select the sample from the sample list. Right click on the sample and select **[Cut]**.
- 4 Select the desired folder, right click on it and select **[Paste]**.

## 6.4 Processing a spectrum

Spectra can be processed or reprocessed using different methods.

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



## NOTICE

There are two types of data collected with Misa depending on the operating procedure used to acquire the data:

1. Standard Data – Data acquired with manual settings or with a STANDARD procedure. These data can only be processed against a STANDARD library with Identification.
2. SERS Data – Data acquired with a SERS operating procedure. These data can only be processed against a SERS library with SERS Identification.

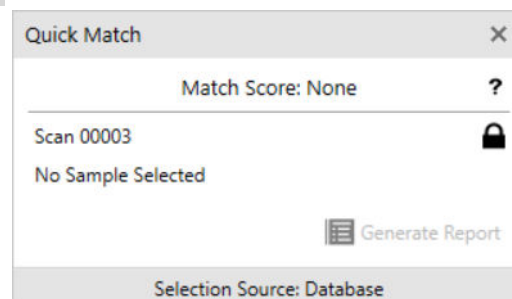
If a data type is processed against a library of a different type, an error message will be displayed.


### Identification – For standard data only

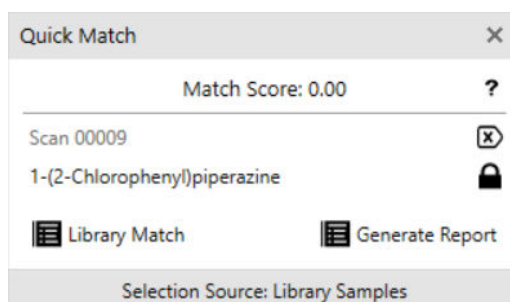
- 1 Select the library to match against from the **Library** selection list.
- 2 Increase or decrease the number in **Matches** to define the number of results shown.
- 3 Increase or decrease the number in **Threshold** to define the threshold for the matching. If the user lowers the number, it will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

### Quick match – For standard data only

- 1 Select **[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.

### SERS identification – For SERS data only

- 1 Select the SERS library to match against from the **Library** selection list.
- 2 Click on **[Match]** to perform the mixture match with the selected parameters.

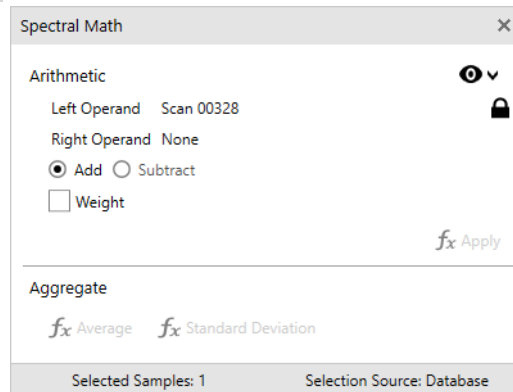
Matches for SERS identification are performed by comparing the location of peaks of the acquired spectrum with the peaks of entries defined in the SERS library.





## Spectral math

On a spectrum, basic spectral math can be performed. These include addition, subtraction, averaging and standard deviation of a set of selected data.

- 1 Click on **[Spectral Math]** to open the **Spectral Math** window.



- 2 Select a spectrum. Press the  icon to lock the active spectrum. Select a different spectrum.
- 3 Chose the math to perform with the 2 spectra. Select multiple spectra for averaging and standard deviation calculations.
- 4 A weighted subtraction or addition can be performed. Activate **Weight** and use the slider or numerical window to adjust the weighted implementation on the operand.
- 5 To see a preview of the results, click on  and activate **Preview Results**.

The result will be displayed in the **Sample** view as a new spectrum.



## NOTICE

Data obtained after Spectral Math operations are treated as STANDARD data.

## 6.5 Generating reports

### Generating sample reports

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

#### Sample report option 1

- 1 Go to the **Sample** view.
- 2 Go to the **Reports** tab.
- 3 Click on either **[Save Summary]** or **[Save Full]**.
- 4 Select a destination for the file. Click on **[Save]**.
- 5 If needed, print out the PDF file.

#### Sample report option 2

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



### NOTICE

Preview the report by selecting either **[View Summary]** or **[View Full]**.

### Generating library reports

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 Go to the **Libraries** view.
- 2 Go to the **Reports** tab.

- 3 Click on **[Save Full]**.
- 4 Select a destination for the file. Click on **[Save]**.
- 5 If needed, print out the PDF file.

### Library report option 2

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



## NOTICE

Preview the report by selecting **[View Full]**.

### Generating operating procedure reports

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 Go to the **Operating Procedure** view.
- 2 Go to the **Reports** tab.
- 3 Click on **[Full]**.
- 4 Select a destination for the file. Click on **[Save]**.
- 5 If needed, print out the PDF file.

### 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.



## NOTICE

Preview the report by selecting **[View Full]**.

## 6.6 Export

### Exporting samples



## NOTICE

Only samples exported with file type **BRMS (.brms)** or **SRMP (.srmp)** can be imported back to Misa Cal. These files are encrypted to protect data integrity. **.brms** is the standard format used in Misa Cal.

**.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 sample to export. Multiple selection is possible.
- 3 Right click on the sample. Click **[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.
- **PRN format (.prn)**  
PRN format (.prn) is a text format.
- **CSV format (.csv)**  
Spectrum CSV format (.csv) is a text format of just plot data.
- **Full CSV format (.csv)**  
Full CSV format (.csv) is a text format that includes metadata.

5 Click on **[Save]**.

### Exporting libraries

- 1 Go to the **Libraries** view.
- 2 Select the library to export. Multiple selection is possible.
- 3 Right click on the library. Click on **[Save As]**. You can save a library only as .lrmf 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 operating procedure to export. Multiple selection is possible.
- 3 Right click on the operating procedure. Click on **[Save As]**. Operating procedures can only be saved as .ormp file type.
- 4 Select a destination for the file. Click on **[Save]**.

### Saving grid data

- 1 Go to the **Samples** view.
- 2 Right click anywhere in the sample list. Click on **[Save Grid Data]**.
- 3 Select a destination for the file. Click on **[Save]**.

### Exporting spectral view image for presentations

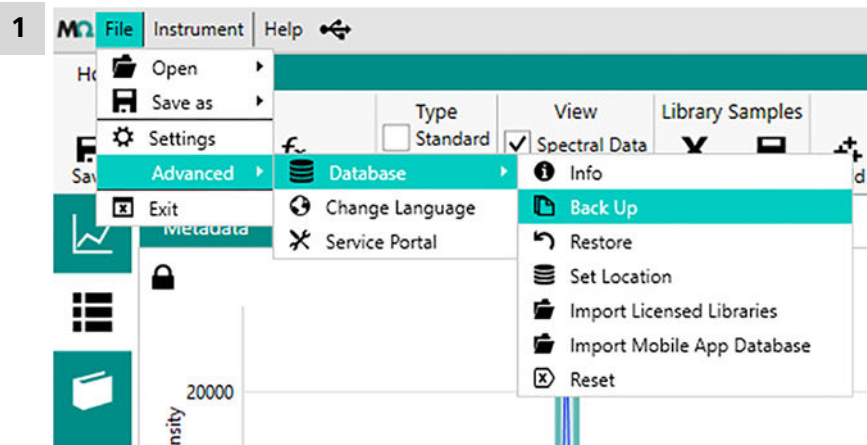
- 1 Go to the **Samples** view.
- 2 Right click anywhere in the sample chart. Click on **[Save Metadata]**.
- 3 Select a destination for the file. Click on **[Save]**.

### Saving baselined data

- 1 Go to the **Samples** view.
- 2 Select a sample. Activate **Baseline** to view baselined data in the viewing window.
- 3 Right click anywhere in the sample chart. Click on **[Save Raw Data]**.
- 4 Select a destination for the file. Click on **[Save]**.

## 6.7 Database backup

### Exporting database



Click on **File ► Advanced ► Database ► Backup**.

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

## Restoring database



### NOTICE

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

An existing Misa Cal 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 on **[Open]**.
- 3 Confirm the restore. Select **[Yes]**.

## 7 Malfunctions and troubleshooting

### 7.1 Creating support log file

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

#### Instrument support log

##### Prerequisite:

A calibration standard is connected.

- 1 Click on **Help ► Create Support File**. Attach the Calibration Standard. Click on **[Okay]**.

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

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



## 8 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 Enter <https://www.metrohm.com/> into your Internet browser.
- 2 Enter the article number of the product (e.g. **2.1001.0010**) into the search field.  
The search result is displayed.
- 3 Click on the product.  
Detailed information regarding the product is shown on various tabs.
- 4 On the **Included parts** tab, click **Download the PDF**.  
The PDF file with the accessories data is created.



### NOTICE

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