Mira Cal

Tutorial

8.105.8020EN

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

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1 Introduction

1.1 Structure of the tutorial

The present tutorial guides you through your first steps using the **Mira Cal** software.

The tutorial concentrates on four parts:

- Prepare the software
- A software description
- Perform measurements
- Create and manage spectra libraries

1.2 Program description

With the Mira Cal software you can conveniently store, manage and exchange data acquired on a Mira spectrometer. The software allows not only to activate/deactivate purchased libraries, but also the data transfer between the Mira spectrometer and the computer and also between different Mira spectrometers.

Using the software you can build your own library and save it on the instrument. This “open library” principle allows you to use the Mira spectrometer in the most flexible way possible.

Available Spectrometer

The following spectrometer can be used with Mira Cal:

- Mira M-1 Basic (User Manual: 8.923.8001)
- Mira M-1 Advanced (User Manual: 8.923.8001)
- Mira M-2 Basic (User Manual: 8.923.8002)
- Mira M-2 Advanced (User Manual: 8.923.8002)

Communication

Communication between the Mira spectrometer and the host computer is established by a USB Mini-B cable.

1.3 Spectral libraries

In addition to the option of creating custom libraries, the following libraries are additionally available and can be purchased:

Table 1 Spectral libraries

Article number	Designation	Number of spectra
6.6071.601	Complete Raman spectral library.	> 8690
6.6071.602	Raman spectra of active substances and auxiliary materials that are relevant to the pharmaceutical industry and medical research.	> 1170
6.6071.603	Raman spectra of solvents.	> 460
6.6071.604	Raman spectra of polymers, polymer additives, plastics, plasticizers and packaging materials.	> 920
6.6071.605	Raman spectra of aliphatic and aromatic aldehydes and ketones.	> 1070
6.6071.606	Raman spectra of alcoholic and phenolic compounds.	> 890
6.6071.607	Raman spectra of esters, lactones and anhydrides.	> 2930
6.6071.608	Raman spectra of hydrocarbons and halogenated hydrocarbons.	> 560
6.6071.609	Raman spectra of chemical substances that are used in the semiconductor industry.	> 370
6.6071.610	Raman spectra of selected hazardous substances that are listed in the "EPA Cameo Database for Chemical Emergencies and Responders" and the "USCG CHRIS Hazardous Chemicals Database".	> 1360
6.6071.611	Raman spectra of selected hazardous substances that are listed in the "EPA Cameo Database for Chemical Emergencies and Responders", "USCG CHRIS Hazardous Chemicals Database", and "NIOSH Guide to Chemical Hazards Databases", as well as chemicals that are regulated by the "Toxic Substances Control Act"	> 3030
6.6071.612	Raman spectra of substances that are relevant to forensic analysis.	> 740
6.6071.613	Raman spectra of pesticides, insecticides, herbicides, fungicides, algicides and similar agricultural chemicals.	> 460
6.6071.614	Raman spectra of selected dyes, colorants, pigments and indicators.	> 300
6.6071.615	Raman spectra of sulfur and phosphorus compounds.	> 970
6.6071.616	Raman spectra of substances with a high production volume, as listed in the "HPV Challenge Program Chemical List".	> 690
6.6071.620	Raman spectra of food additives, including FDA-controlled substances. Additionally, spectra of indirect food additives and substances that come into contact with foodstuffs, such as packaging materials and associated processing chemicals.	> 1070

Article number	Designation	Number of spectra
6.6071.621	Raman spectra of biochemicals, including vitamins, resins, starches, glycerins, fatty acids, sugars, carbohydrates, proteins, and peptides.	> 1900
6.6071.622	Raman spectra of flavors, scents, and other substances that are used for manufacturing cosmetics.	> 1030

1.4 Symbols and conventions

The following icons and formatting are used in this documentation:

1	**Instruction step** Carry out these steps in the sequence shown.
Method	**Dialog text**, **parameter** in the software
File ▸ New	Menu or menu item
[Continue]	**Button** or **key**
	**WARNING** This symbol draws attention to a possible life-threatening hazard or risk of injury.
	**Note** This symbol highlights additional information and tips.

2 Preparation

2.1 Install the software

Check System requirements

1 Make sure, the used system fulfils the system requirements *(see Chapter 7, page 31)*.

Check Windows User rights

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

2 Make sure, that User rights settings are set to „Always notify“ or „Notify me only when programs try to make changes to my computer“.

NOTE

This step depends on the installed operating system and gis described here:

https://support.microsoft.com/en-us/kb/975787

Install the software

1 Double-click on „Mira_Cal.exe“.

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

Install spectrometer driver.

1

NOTE

As soon as the spectrometer connects for the first time, the driver for the spectrometer is installed automatically. Therefore an internet connection is needed.

2 If the installation was not successful:

- **A**: Open Mira Cal*(see Chapter 2.2, page 5)*.
- **B**: Go to **File** ▸ **Advanced Updates** ▸ **Install** ▸ **Device Drivers**.

2.2 Start the software

1

NOTE

As soon as the software is installed, Mira Cal icon appears on the desktop of the computer.

Double-click on , to start the program.

2.3 Establish connection

Physically connect the spectrometer to the host

1 Connect the spectrometer to the PC using the USB Mini-B cable.

2 Turn on the instrument and enter the PIN code (default: 1234) (see instrument user manual *"Spectrometer variants", Page 1*).

Connect the spectrometer with Mira Cal

1

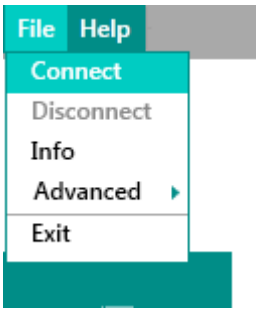


Figure 1 Menu item „Connect“

In Mira Cal choose Menu item **File** ▸ **Connect**.

2 Click on **[Refresh]**.

The spectrometer is listed in „Available COM Devices“.

NOTE

If the spectrometer is not listed, repeat step 2 until it is listed.

3

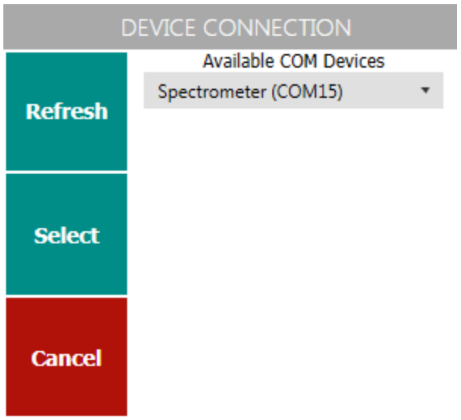
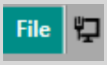


Figure 2 Dialog box „Device Connection“

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

NOTE

A successful connection is indicated by the icon 

in Mira Cal and the icon  on the screen of the spectrometer.

Disconnect the spectrometer

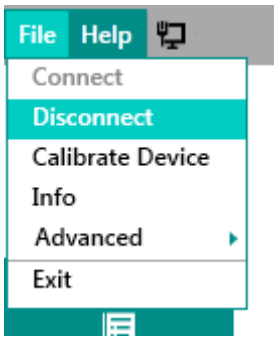
1 

Figure 3 Menu item „Disconnect“

Click on **File** ▸ **Disconnect**, to disconnect the spectrometer.

2 Disconnect the USB Mini-B cable from the computer.

2.4 Firmware Update

NOTE

After a Firmware Update, the instrument must be calibrated again. Information regarding calibration can be found in the user manual of the instrument.

NOTE

When you installed a new version of Mira Cal, make sure to update the instruments firmware as well.

Update spectrometer firmware

1

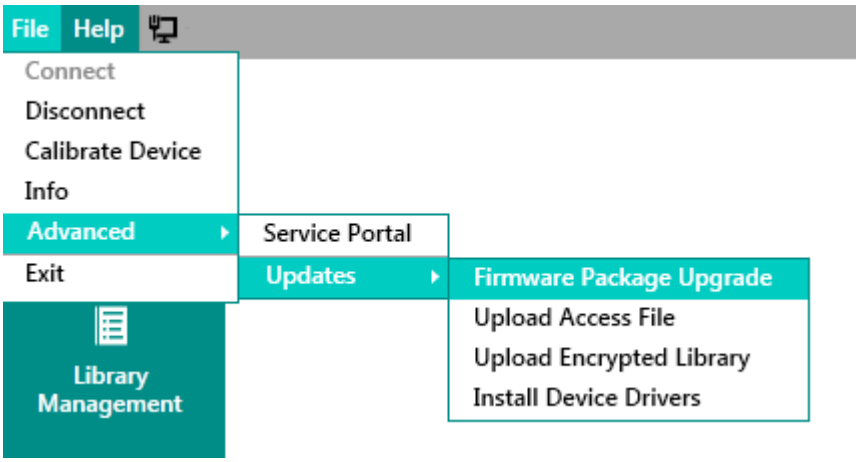


Figure 4 Menu item „Update Firmware“

Click on **File** ▸ **Advanced** ▸ **Updates** ▸ **Update Firmware**.

Figure 5 Dialog box „Update Device Firmware“

The dialog box „Update Device Firmware“ opens.

2 Click on **[Update]**, to update the firmware.

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

2.5 Update S.T. Japan Library

The Mira-spectrometer is delivered with a full, inactive set of S.T. Japan libraries.

A library update is only needed if an updated set of S.T. Japan libraries will be installed (for example if more spectra or libraries are available.

Please contact your Metrohm representative for further information.

Load a library to the spectrometer

Make sure, a spectrometer is connected.

1

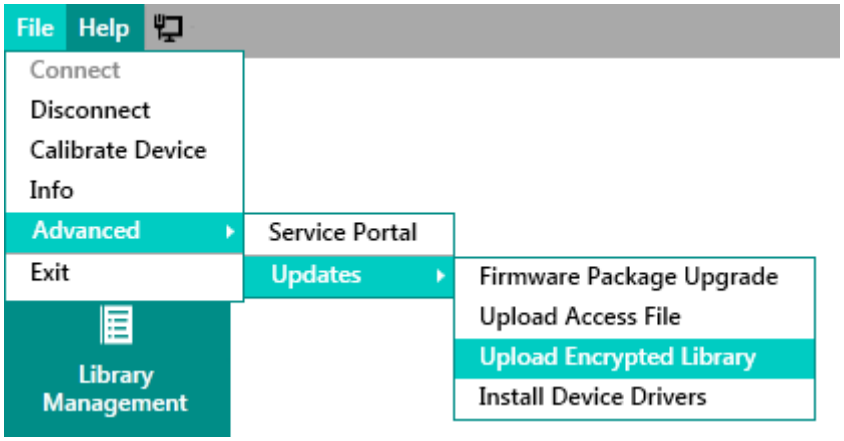


Figure 6 Menu item „Upload Encrypted Library“

Click on **File** ▸ **Advanced** ▸ **Updates** ▸ **Upload Encrypted Library**.

2 Select the .zip file with the new library and click on **[Open]**.

The library will be loaded to the spectrometer. Subsequently the spectrometer will reboot automatically.

NOTE

The reboot can last several minutes. Do not disconnect the spectrometer within the reboot.

3 Activate library *(see Chapter 5.2, page 27)*.

3 Software description

3.1 Overview

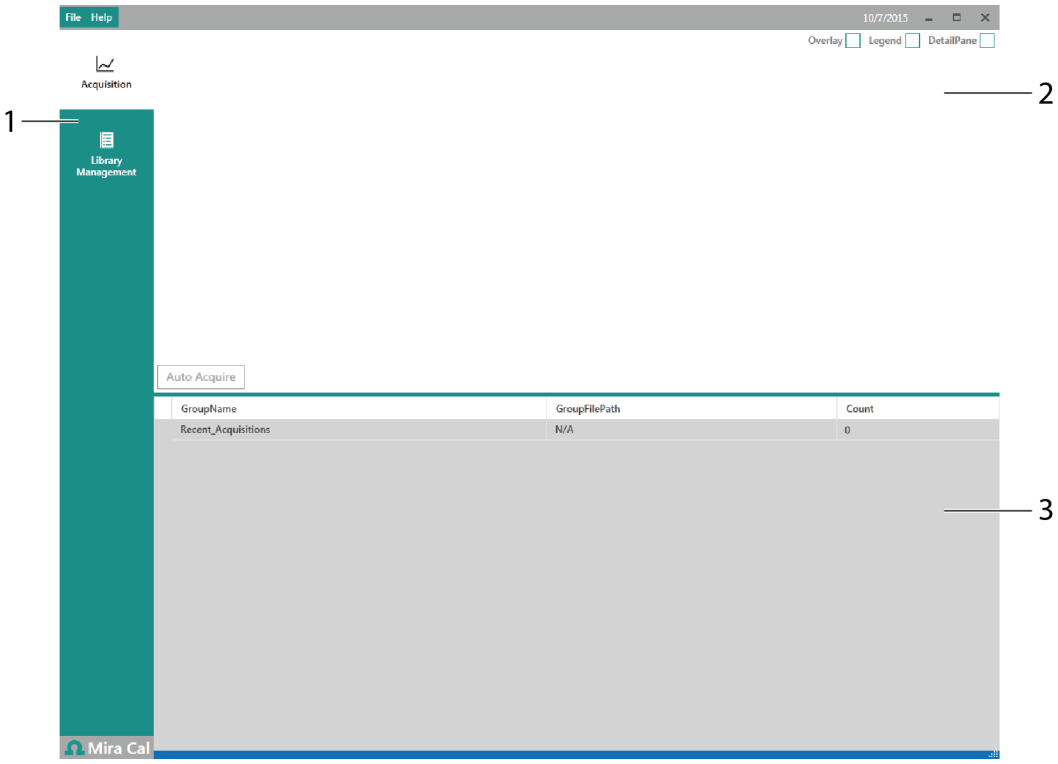


Figure 7 Overview graphic

1 Menu items	**2 Spectra view**
3 Sample list	

Table 2 Description

Menu items	Buttons to select between the menu items „Acquisition“ and „Library Management“ *(see Chapter 3.2, page 11)*.
Spectra view	The Spectra Viewer is used for visual inspections of gathered spectra. The spectrum of the sample is displayed in blue. A matching library spectrum is shown in green as soon as the library is selected. *(see Chapter 4.1, page 18)*.

Sample list	The sample list contains information about the collected samples (for example date and time). Spectra are divided in groups and can be opened by clicking on the triangle ▷ left of the group name. Possible matches with a library, can be opened by clicking on the triangle ▷ left of the spectrum name.

3.2 Menu items

Mira Cal has two different program parts which can be opened by clicking on the corresponding menu item symbol in the vertical bar on the left.

The menu item symbol for the opened program part is shown in white with black icons. The symbols for the other program part in green with white icons.

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

Menu item „Acquisition“

Figure 8 Menu item „Acquisition“

- Spectra view (with **Overlay** and **DetailPane**).
- Acquire samples with remote controlling via Mira Cal.
- Match measured spectra to device library.
- Save and load acquired spectra to and from a local drive.
- Generate reports.

Menu item „Library Management“

Figure 9 Menu item „Library Management“

- Download libraries from Mira spectrometer to PC and import measured spectra.
- Create custom libraries.
- Add/remove substances from libraries.

- Upload changes to the connected Mira spectrometer.
- Manage libraries of connected Mira spectrometer.

3.3 Spectra view

Spectra view is a tool for visual inspection of acquired spectra. Spectra View can be used to load and display spectra in different formats (*.rmn, *.spc, *.txt).

Copy displayed spectrum to clipboard

The currently displayed spectrum can be copied to the clipboard.

1 Right-click into the Spectra View.

2

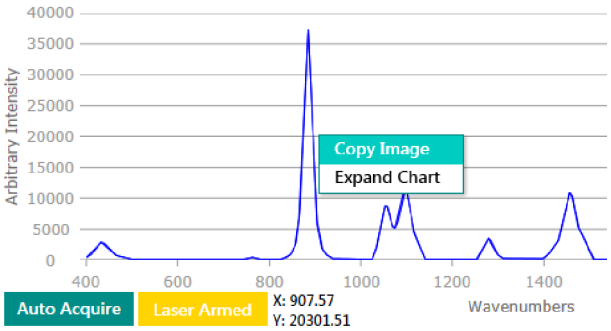


Figure 10 Context menu

Click on **Copy Image** in the dialog box.

Zoom and DetailPane

Zoom

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

2

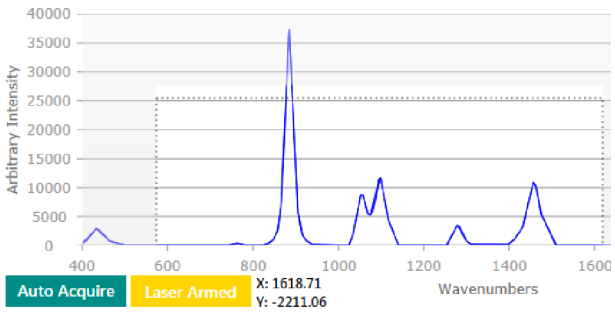


Figure 11 Zoom

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.

DetailPane

1

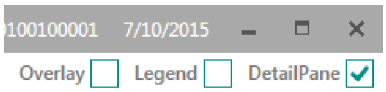


Figure 12 Selection „Detail Pane“

Mark check box „DetailPane“.

2

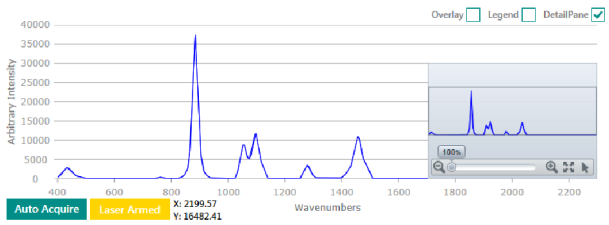


Figure 13 Window „Zoom“

The opening window zooms into displayed spectrum.

NOTE

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

3 Click on  to get back to original size.

Overlay spectra

1

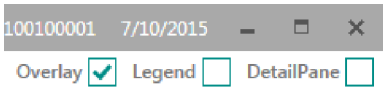


Figure 14 Selection „Overlay“

Mark Check box „Overlay“ that spectra can be overlayed.

Spectra can be selected to display the names.

NOTE

A multiple selection of spectra is possible.

Display legend

1

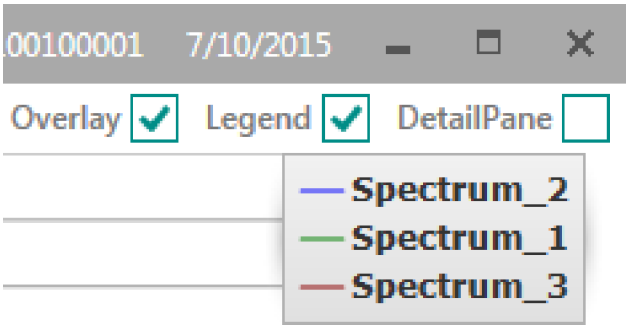


Figure 15 Selection „Legend“

Mark Check box „Legend“ to display the legend.

3.4 Sample list

The sample list displays the current loaded spectra.

These are divided in groups and come from measurements with Mira and Mira Cal, or have been loaded from a local hard drive.

3.4.1 Save spectra

Spectra can be saved in three different spectral formats:

- **RAMAN (.rmn)**
  This is the standard format used in Mira Cal. 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*.

Save data to the local drive

1 Right-click on the group or spectrum of choice.

NOTE

A multiple selection of several groups is possible.

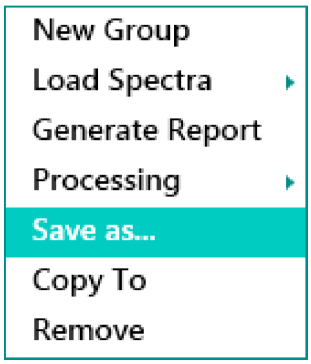
2 

Figure 16 Context menu

Click on **Save As...** in the opening context menu.

3 In the dialog box select the file format and file location and click on **[Save]**.

3.4.2 Load spectra

Spectra in the above file formats can be loaded for visual inspections and transfer to libraries.

Load spectra from the local drive

1 Right-click on the Sample list pane.

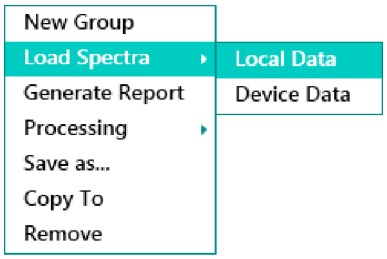
2 

Figure 17 Context menu

Choose **Load spectra ▸ Local data** from the context menu.

3 From the appearing dialog box choose the spectra to be loaded and click on **[Open]**.

3.4.3 Manipulate spectra

Average spectra of a group

1 Right-click on a spectrum.

NOTE

A multiple selection of spectra is possible.

2 In the context menu, click on **Processing** ▸ **Average Selected**.

The spectrum is added to the group „Averages“.

3 If needed, edit the name of the group.

3.4.4 Generate reports

Generate a PDF report.

1 Right-click on the desired spectrum.

NOTE

A multiple selection of spectra is possible.

2

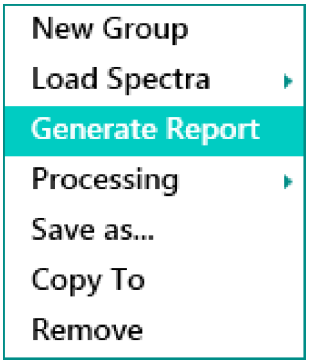


Figure 18 Context menu

In the context menu click on **Generate Report**.

3 In the dialog box select the file format and file location and click on **[Save]**.

4 Data acquisition

There are two ways of analyzing samples and acquiring spectra.

First by using the Mira spectrometer only, and alternatively by remote controlling via Mira Cal.

4.1 Data acquisition with Mira

Acquire data

NOTE

Refer to Mira User Manual *(see "Available Spectrometer", page 1)* for detailed description of the following steps:

1 Acquire spectra.

2 Save acquired spectra.

Transfer acquired spectra from Mira to Mira Cal

1 In Mira Cal select menu item **Acquisition**.

2 Right-click in the Sample list.

3

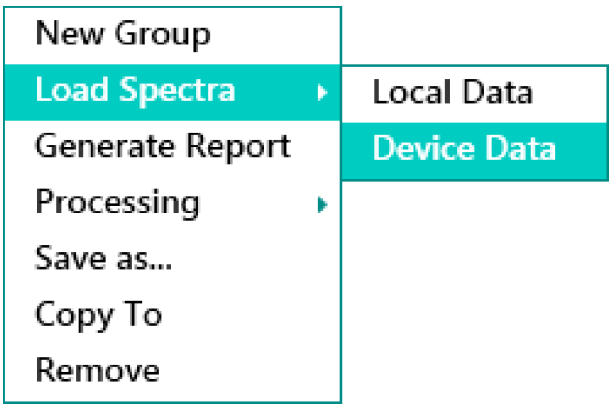


Figure 19 Context menu

Click on **Load Spectra** ▸ **Device Data** in the context menu.

4

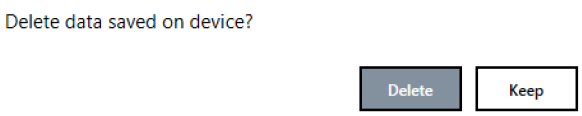


Figure 20 Dialog box „Delete Data“

Click on **[Delete]** to delete Spectra from spectrometer or click on **[Keep]** to keep data on the spectrometer.

The spectra can be found in a new group called “Import from Instrument“.

4.2 Data acquisition with Mira Cal

Acquire data

1 Connect computer to an instrument *(see Chapter 2.3, page 5)*.

2 Select menu item „Acquisition“.

3 Position the sample for measurement.

NOTE

Refer to the Mira user manual *(see "Available Spectrometer", page 1)* for detailed description.

4

WARNING

Risk of injury by laser radiation

The Mira Advanced spectrometer are class 3B laser which can emit laser light during data acquisition.

The laser radiation can cause serious eye injuries if the safety measures are not followed.

- The provided protective glasses must be worn when using an attachment lens.
- The safety regulations must be observed (refer to Mira user manual *(see "Available Spectrometer", page 1)*).

When the laser is armed, pressing **[Auto Acquire]** will fire it. Arming the laser is not required before each measurement.

Figure 21 Arming Laser

1 Button „Arm Laser“

When using a Mira Advanced, click on **[Arm Laser]** *(21-**1**)* to arm the laser.

5

Figure 22 Starting the measurement

2 Button „Auto Acquire“

Click on **[Auto Acquire]** *(22-**2**)* to start measurement.

The sample is now listed in the group „Recent Acquisitions“.

6

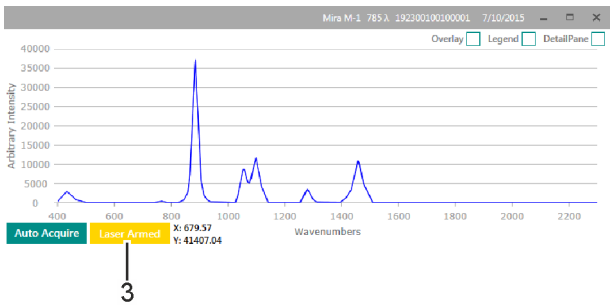


Figure 23 Disarm Laser

3 Button „Laser Armed“

Click on **[Laser Armed]** *(23-**3**)* to disarm the laser.

5 Spectral libraries

NOTE

A spectrometer must be connected in order to perform the following operations.

5.1 Create and manage custom libraries

NOTE

Custom libraries are built from measurements of user samples. It is of utmost importance that these samples are representative of the statistical population. Failing to select appropriate samples will lead to poor performance of the library matching. Consider measuring many samples and average the spectra.

5.1.1 Create and load local libraries

Create a new library

1 Select menu item „Library Management“.

2

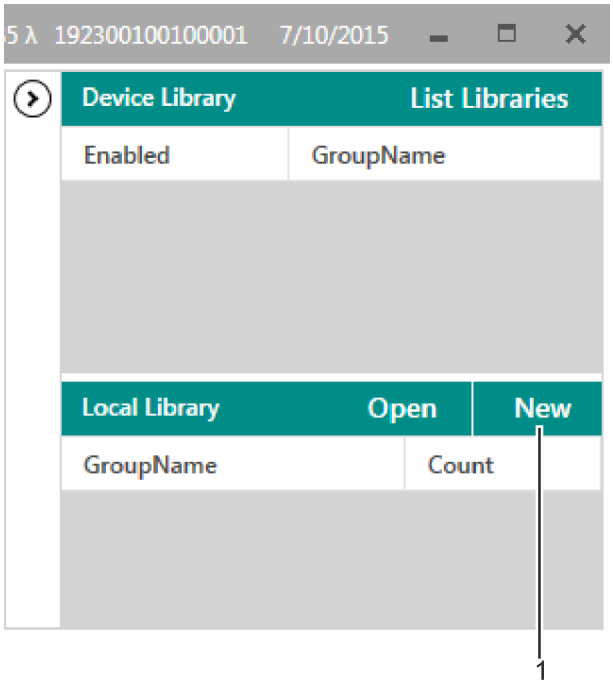


Figure 24 Button „New“

In the „Local Library“ section click on **[New]**.

3 Rename the new library.

Load a library

1 Select menu item „Library Management“.

2

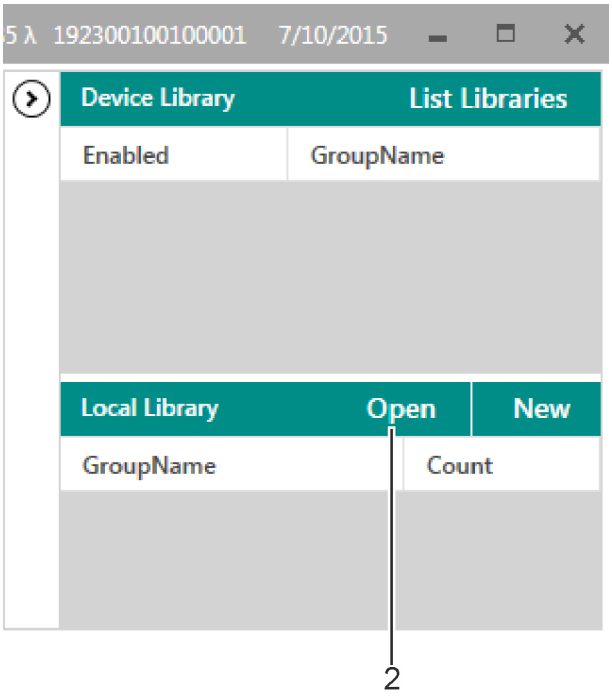


Figure 25 Button „Open“

In the „Local Library“ section click on **[Open]**.

3 Select the desired library and click on **[Select Folder]**.

5.1.2 Modify libraries

Add sample to a library

1 Select menu item „Acquisition“.

2 Acquire or load data.

3 In the Sample list, right-click the sample or the group you want to add.

4

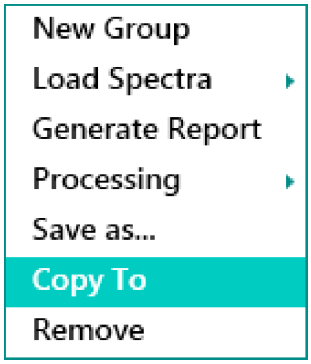


Figure 26 Context menu

Click on **Copy to...** in the context menu.

5

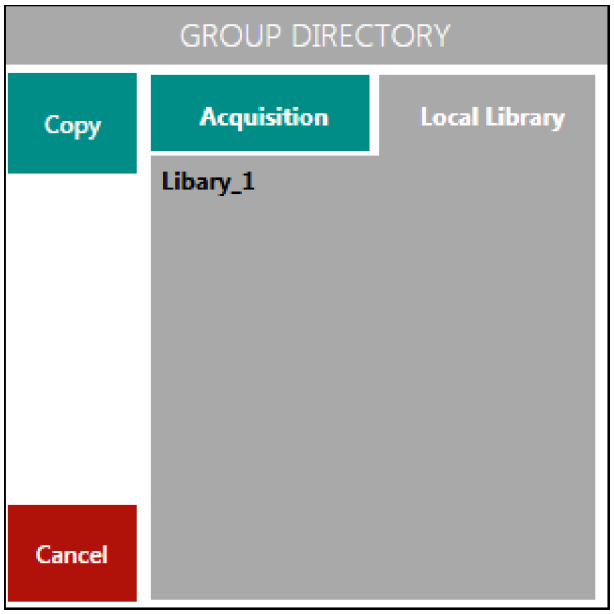


Figure 27 Dialog box „Group directory"

Select the library you want to add the spectrum to and click on **[Copy]**.

Remove samples from a library

1 Select menu item „Library Management".

2 Select the desired library with the sample you want to delete.

3 In the Sample list right-click on the sample you want to remove.

4

Figure 28 Context menu

Click on **Remove** in the context menu.

Save library local

1 Select menu item „Library Management“.

2 In „Local Library“ right-click on the library you want to save.

3

Figure 29 Context menu

Click on **Save As...** in the opening context menu.

4 Choose the file location and click on **[Save]**.

NOTE

It is recommended to always save libraries in the .rmn format.

5.1.3 Upload library to spectrometer

1 Select menu item „Library Management“.

2 Right-click on the library you want to upload to the spectrometer.

3 Click on **Upload to Device** in the context menu.

5.2 Activate S.T. Japan libraries

Buy library

To purchase libraries, contact your local Metrohm representative. You will be provided with an activation file.

Activate library

The spectrometer must be connected.

1

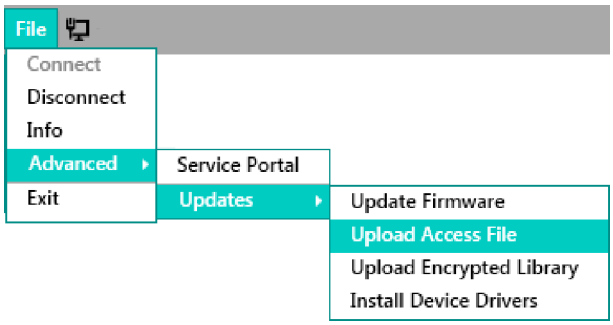


Figure 30 Menu item „Upload Access File“

Click on **File** ▸ **Advanced** ▸ **Updates** ▸ **Upload Access File**.

2 Choose the file and click on **[Open]**.

5.3 Enable or disable libraries for search

NOTE

- The fewer libraries are activated for the spectral comparison, the shorter the search.
- If many libraries are activated, the sample may have a high match rate for several library substances and thus be difficult to identify.
  It is advisable to incorporate previous knowledge of the sample into the identification.
  For this reason, the libraries are arranged according to subjects. We recommend activating only those substance classes that fit the sample.
- It is recommended not to use libraries with big and small data at the same time.
- The settings described in this chapter only determine whether a library is included in the search or not.
  Newly purchased libraries first have to be activated in the Mira Cal.

Libraries can be enabled /disabled either directly on the spectrometer or using Mira Cal.

Enable or disable libraries on the spectrometer

1 Refer to the Mira user manual *(see "Available Spectrometer", page 1)* for a detailed description how to enable or disable libraries on the spectrometer.

Enable or Disable libraries using Mira Cal

1 Select menu item „Library Management“.

2 Click on **[List Libraries]**.

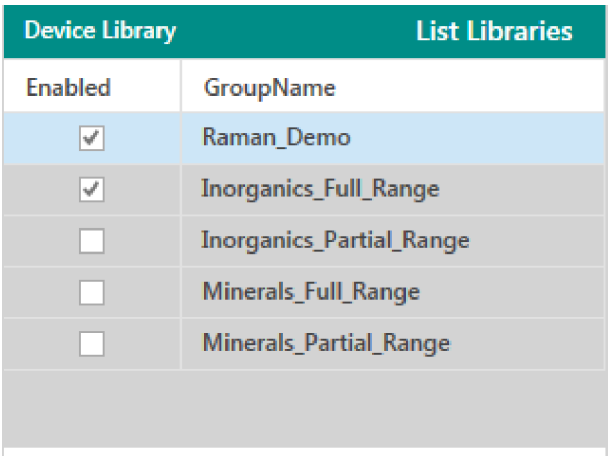


Figure 31 Dialog box „Device Library“

The dialog box „Device Library“ opens.

NOTE

All libraries are listed. The checkbox in the „Enabled“ column indicates, whether libraries are enabled for search or not.

3 Right-click on a library.

4

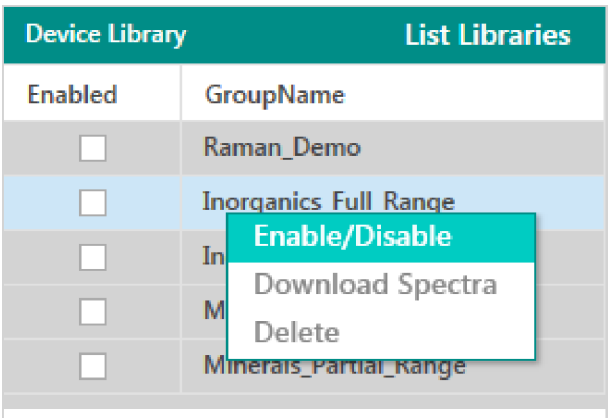


Figure 32 Context menu

Click on **Enable** in the context menu, to enable the library for search or click on **Disable** to disable the library for search.

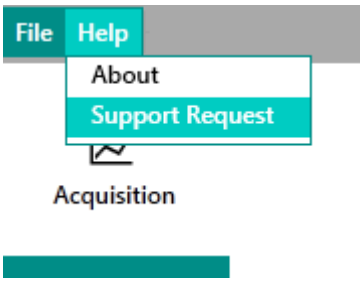
6 Troubleshooting

6.1 Support Request

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.

1 Click on **[Help]**.

2 Click on **[Support Request]**.



3 Choose file location

7 System requirements

Processor	Pentium 4 equivalent or higher
Operating system 32 or 64 bit version of:	▪ 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, two free ports 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

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