MIRA Cal DS

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Tutorial

8.105.8069EN / 2021-09-15

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1.2.50

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1 Overview

1.1 Product description

MIRA Cal DS software is used together with the Metrohm Instant Raman Analyzers MIRA XTR DS / MIRA DS.

MIRA Cal DS software

- Administration
  - For example users, operating procedures
- View results
- Generate reports
- Store all data

MIRA XTR DS / MIRA DS instruments

- Analyze samples

Synchronization between MIRA XTR DS / MIRA DS instruments and MIRA Cal DS software

With the help of a synchronization workflow, all needed data is synchronized between MIRA Cal DS software and MIRA XTR DS / MIRA DS instruments.

Synchronizing MIRA XTR DS / MIRA DS instruments to MIRA Cal DS software ensures that the instrument is up to date. The current versions of active operating procedures, libraries and user accounts are transferred to the instrument. Samples are saved to the database.

More than 1 instrument can be used. They can be synchronized to the same database in order to achieve a clean data management.

Evaluation

In MIRA Cal DS software, an evaluation option is available:

- Identification of samples:
  The measured spectrum of a substance is compared with existing spectra in a library. Results for both library identification and mixture matching can be obtained.

1.2 Product versions

The product is available in the following version:

Order number	Designation	Version feature
6.06071.020	MIRA Cal DS	Version 1.2.50

1.3 Symbols and conventions

The following formatting may appear in the documentation:

*(5-**12**)*	Cross-reference to figure legend The first number refers to the figure number. The second number refers to the product part in the figure.
1	Instruction step Numbers indicate the order of the instructions steps.
Method	Names of parameters, menu items, tabs and dialog windows
File ► New	Menu path
[Continue]	Button or key

1.4 Additional information – Device manuals

Refer to the following manuals for information about the instruments:

- Manual MIRA DS: 8.926.8001EN
- Manual MIRA XTR DS: 8.0926.8005EN

Insert the product number into the search field on *https://www.metrohm.com* to find the manuals.

2 Safety

2.1 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.

2.2 Responsibility of the operator

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

- Instruct personnel in the safe handling of the product.
- Train personnel in the use of the product according to the user documentation (e.g. install, operate, clean, eliminate faults).
- Train staff on basic occupational safety and accident prevention regulations.
- Provide personal protective equipment (e.g. protective glasses, gloves).
- Provide suitable tools and equipment to carry out the work safely.

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

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

2.3 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.

2.4 Safety instructions

2.4.1 Danger from electrical potential

WARNING

Electric shock from electrical potential

A considerable danger of injury exists in connection with touching live parts.

- Never open the housing of the instrument when the power cord is connected. You can not service or replace any parts inside the housing.
- Only personnel who have been issued Metrohm qualification may perform service and repair work on electric and electronic parts.
- The electrical safety of the instrument is ensured as part of the international standard IEC 61010.

2.4.2 Danger from radiation

WARNING

Eye injury by laser radiation

Laser radiation can cause serious eye injuries.

- Follow the safety measures and instructions.
- Instruments must be used by trained personnel only.
- Instruments of the laser class 3B must be used in protected and labeled rooms only.
- When working with open laser beams (Smart Tips of the laser class 3B) appropriate protective glasses must be used, see chapter "Operating specifications" in the MIRA device manuals.
- Observe the nominal ocular hazard distance (NOHD).
- Follow the provisions of the IEC 60825-1 standard "Safety of laser products" and the regulations for the use of laser systems in your country.

2.5 Design of warning messages

There are 4 hazard levels for warning messages. The following signal words are used for classifying the hazard levels in warning messages:

- **DANGER** indicates a hazardous situation which, if not avoided, will result in serious injury or death.
- **WARNING** indicates a hazardous situation which, if not avoided, could result in serious injury or death.
- **CAUTION** indicates a hazardous situation which, if not avoided, could result in minor or moderate injury.
- **NOTICE** indicates a hazardous situation which, if not avoided, could result in property damage.

Warning messages differ in design (color and warning sign) depending on the hazard level:

DANGER

Type and source of danger

Consequences when not observing the notice: An irreversible injury that may result in death is very probable.

- Measures to avoid the danger

WARNING

Type or source of danger

Consequences when not observing the notice: A serious injury that may result in death is probable.

- Measures to avoid the danger

CAUTION

Type or source of danger

Consequences when not observing the notice: A minor to moderate injury is probable.

- Measures to avoid the danger

2.6 Meaning of warning signs

This documentation uses the following warning signs:

Table 1 Warning sign according to ISO 7010

Warning sign	Meaning
	General warning sign
	Warning of electrical voltage
	Warning of hand injuries
	Warning of sharp object
	Warning of hot surface
	Warning of biological hazard
	Warning of toxic materials

Warning sign	Meaning
	Warning of flammable materials
	Warning of corrosive substances
	Warning of optical radiation
	Warning of laser beams

Depending on the intended use of the product, the corresponding warning sign stickers must be placed on the product.

3 Functional description

3.1 General overview

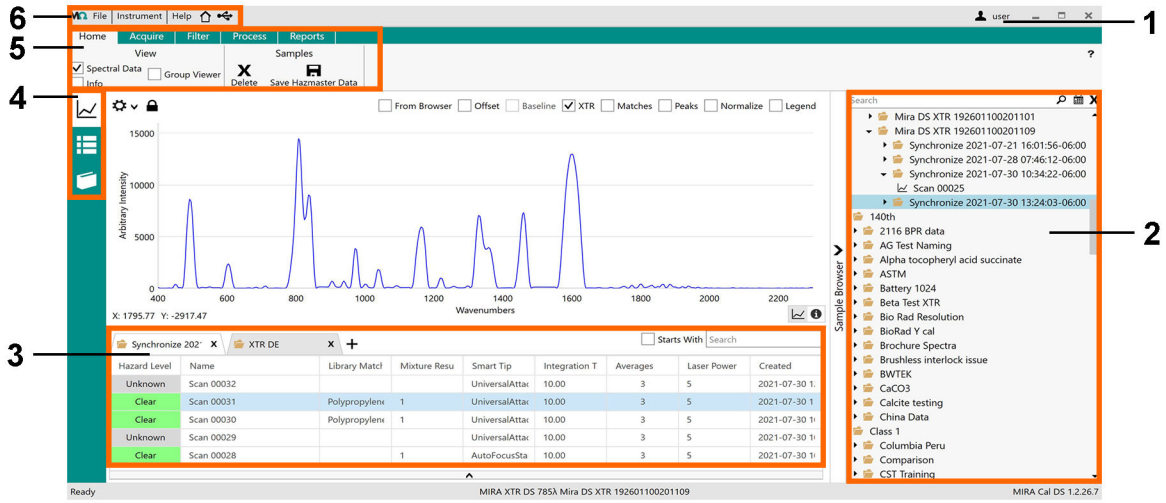


Figure 1 MIRA Cal DS – General overview

1	**Logged in user**	**2**	**Sample browser**
3	**Sample viewer** with sample lists	**4**	**Function tabs** Sample view Library view Operating procedure view
5	**Ribbon**	**6**	**Menu bar**

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.

MIRA XTR DS / MIRA DS has a **Smart Acquire** feature which automatically optimizes the acquisition parameters for a sample.

Users can also build operating procedures by using parameters that the user selects, either in the MIRA Cal DS software or on the MIRA XTR DS / MIRA DS instrument. Operating procedures can be shared between MIRA XTR DS / MIRA DS instruments.

3.3 Drop down menus

File	
Open ►	
Samples	Imports samples.
Libraries	Imports libraries.
Operating Procedures	Imports operating procedures.
Save As ►	
Samples	Saves samples to selected location.
Libraries	Saves libraries to selected location.
Operating Procedures	Saves operating procedures to selected location.
Settings	Opens a view with two tabs: ▪ General *(see "General tab", page 11)* ▪ Reports *(see "Reports tab", page 13)*
Advanced ►	
Database	▪ **Info** Lists database information. ▪ **Help** ▪ **Back Up** Backs up the database. ▪ **Restore** Restores the database. ▪ **Set Location** Sets the location of the database. ▪ **Import Licensed Libraries** Imports licensed libraries ▪ **Import MIRA Cal M Database** Imports the database from MIRA Cal M. ▪ **Reset** Removes all items from the database, including operating procedures, samples and libraries.
Change Language	Changes the language of the application.

Manage Advanced Users	Changes the user password, manages and reviews users (only visible if **[Require Advanced Login]** is checked in **Settings**).
Service Portal	Allows access for service engineer.
Exit	Closes MIRA Cal DS.

Instrument	
Connect	Connects MIRA XTR DS / MIRA DS to MIRA Cal DS.
Disconnect	Disconnects MIRA XTR DS / MIRA DS from MIRA Cal DS.
PIN codes	The user can add PIN codes. Double click a PIN code entry to delete, enable or disable a PIN code. The default PIN code is 1234. It cannot be edited or deleted.
Bluetooth PIN code	Is displayed only when the MIRA XTR DS / MIRA DS instrument is connected to MIRA Cal DS. Change the PIN code for the Bluetooth® wireless connection with MIRA Cal M. The default PIN code is 9999.
System Suitability Test Archive	Lists all system suitability tests in the database.
Info	Lists identification information of the instrument and the operating system.
Rename	Is displayed only when the MIRA XTR DS / MIRA DS instrument is connected to MIRA Cal DS. The user can change the name of MIRA XTR DS / MIRA DS.
Full Sample Download	Downloads all samples stored on MIRA XTR DS / MIRA DS.
Execute Script	Allows the user to execute service scripts for minor adjustments to MIRA XTR DS / MIRA DS.
Calibrate Instrument	The user will be prompted throughout the calibration routine. System suitability test can be run immediately following calibration.
System Suitability Test	The test can be run independently of the calibration routine. Follow the prompts. Prompts the user through the system suitability test routine. Runs system suitability test independently of calibration routine.
Updates ►	

Upload Language Package	Updates languages for the application.
Upload Certificate Package	Updates licensed libraries.
Advanced	Is displayed only when MIRA XTR DS / MIRA DS is connected to MIRA Cal DS. ▪ **Upload Encrypted Library** Uploads an encrypted library. ▪ **Upload Library Access File** Uploads a library access file. ▪ **Upload S.T. Japan** Uploads an S.T. Japan library.

Help	
About	Displays the MIRA Cal DS version and copyright.
Create Support File	Generates a support file for the desktop software and MIRA XTR DS / MIRA DS. The user will be asked to attach the Calibration Standard and select **[Okay]**. A support file is generated and the user is prompted to save the file. The support file can be sent to Metrohm Raman should there be issues with the device or desktop software.

Home	Click on and the user is returned to the home screen.

Connected	Displays when MIRA XTR DS / MIRA DS is connected to MIRA Cal DS.

General tab

File ▶ Settings

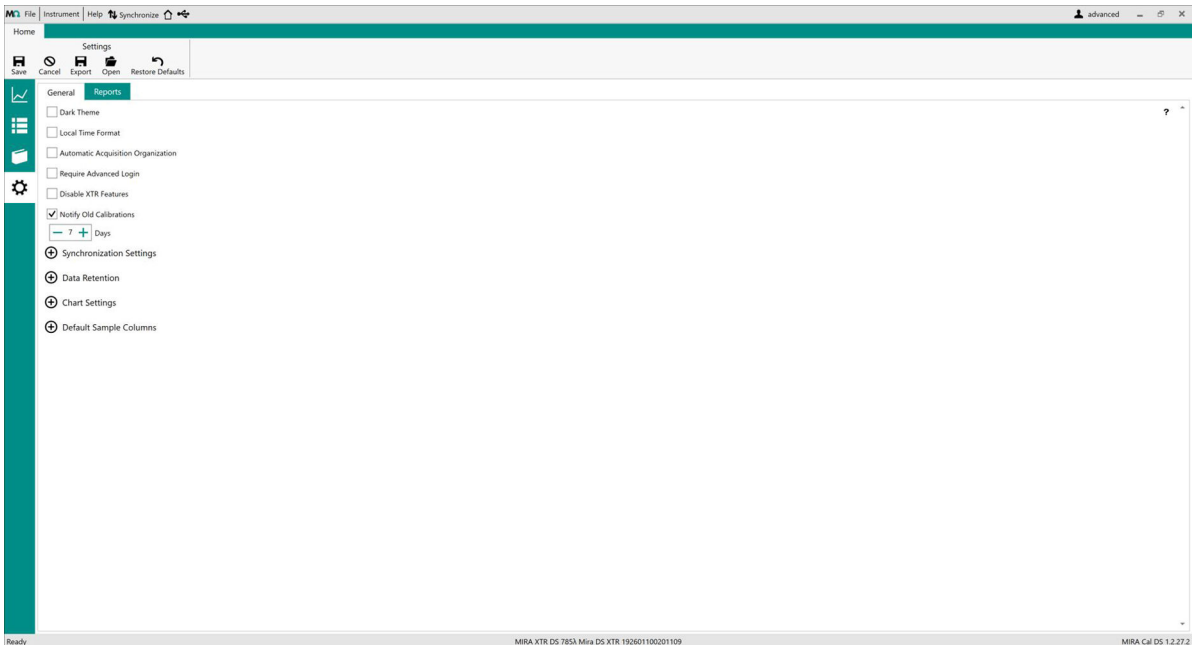


Figure 2 Settings - General tab

In the General tab you can set the following:

General tab	
Dark Theme	Sets the software background to the color black.
Local Time Format	Sets the time to the local computer format.
Automatic Acquisition Organization	Automatically creates a folder with the serial number of MIRA XTR DS / MIRA DS and with the time and date when acquisitions are performed by MIRA Cal DS.
Require Advanced Login	Requires the user to login to use the advanced features of the software (*see "Managing users", page 52*). ▪ Check **Require Advanced Login**. ▪ Change the password for the default advanced user by entering a password and click **[Change]**. ▪ Add a new user by entering the user name and password and click **[Save]**. ▪ Delete users by selecting the user from the **Delete Users** window and click **[Delete]**. ▪ Click **[Close]**. ▪ Go to the **Home** ribbon and select **[Save]**.
Disable XTR Features	Hides XTR features in the software.
Notify Old Calibrations	Gives a pop up reminder if the time since the last calibration is longer than the set time period.
Synchronization Settings ►	

Save Sample Summary On Sync	Saves sample summary after synchronization.
Save System Suitability Test On Sync	Saves system suitability test after synchronization.
Auto Synchronize	Automatically synchronizes to the device and/or database after a modification of operating procedure, library or other device modification. The synchronization of user operating procedures, licensed libraries and user libraies can be checked separately.
SmartSync	A custom folder can be set for device synchronization. The custom folder can be defined by: Day, Device Name, Serial Number, Sync Time, Hazard Level, PIN code, or Operating Procedure.
Data Retention ►	
Retain All Data	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.
Chart Settings ►	
Y Grid Lines	Displays Y grid lines in the sample chart.
X Grid Lines	Displays X grid lines in the sample chart.
Invert X Axis	Inverts X axis in the sample chart.
Chart Line Thickness	Defines chart line thickness.
Default Sample Columns	Defines the sample columns displayed in the **Sample** view.

Reports tab

File ► Settings

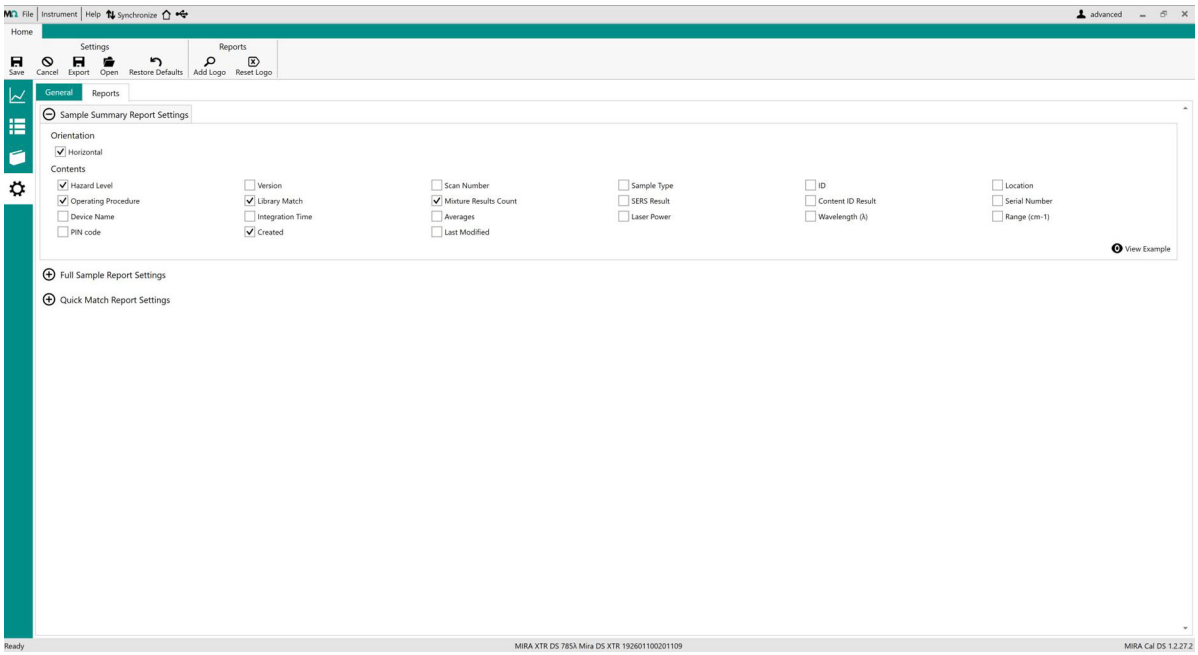


Figure 3 Settings - Reports tab

In the Reports tab you can set the following:

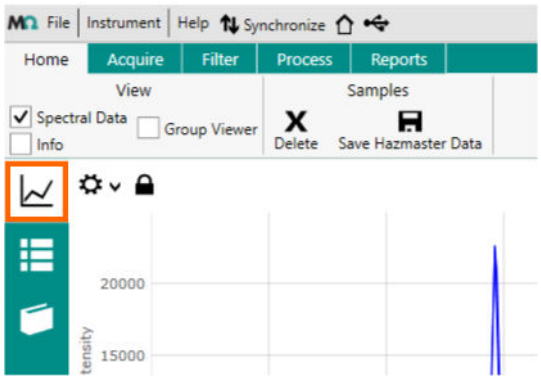
Reports tab	
Sample Summary Report Settings	The selected settings define the content of the **Sample Summary** report. Click on **View Example** to view, save or print the report. To add a personalized logo to the report, click on **Add Logo** in the **Reports** section of the **Home** tab.
Full Sample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

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
- **Synchronize** view

Sample view



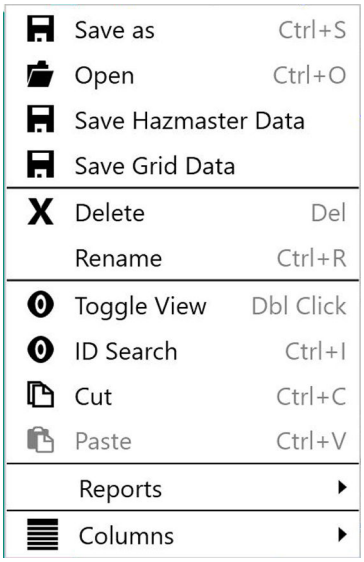
Sample

Home ▶

Samples

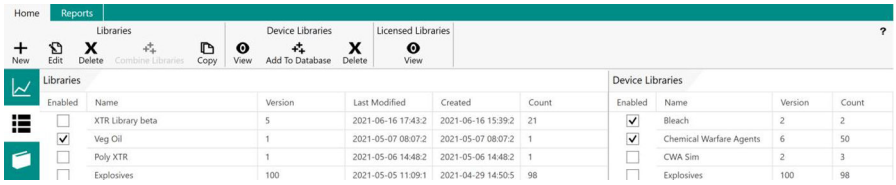
Click on a sample in the sample list to highlight and carry out actions.

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

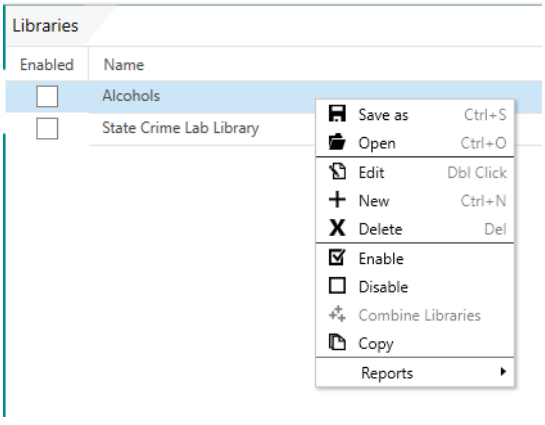


Acquire ▶	Is displayed only when the MIRA XTR DS / MIRA DS instrument is connected to the MIRA Cal DS software.
Acquisition Settings	Select acquisition settings for scanning a sample while MIRA XTR DS / MIRA DS is connected to MIRA Cal DS (*see "Data acquisition with MIRA XTR DS / MIRA DS", page 41*).
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. ▪ **Mixture Identification** Perform mixture matching against the chosen library (use 0.999 to force a mixture match). ▪ **Spectral Math** Add or subtract two spectra or perform other mathematical operations on selected data.
Reports	Generate reports for the selected spectra.

Library view

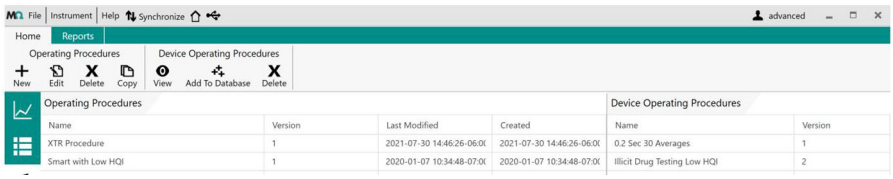


Library 	
Home ▶	
Libraries	Right click on a selected library to open a function menu.

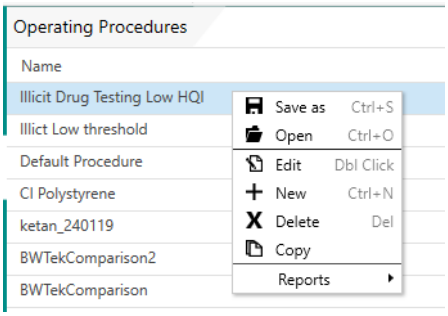


Libraries	Displays the libraries on the device. Libraries can be added to or removed from the device.
Licensed Libraries	Select a licensed library and click on **View** to see the contents of the library.
Reports ►	
Library Reports	Generate reports for the selected libraries.

Operating procedure view

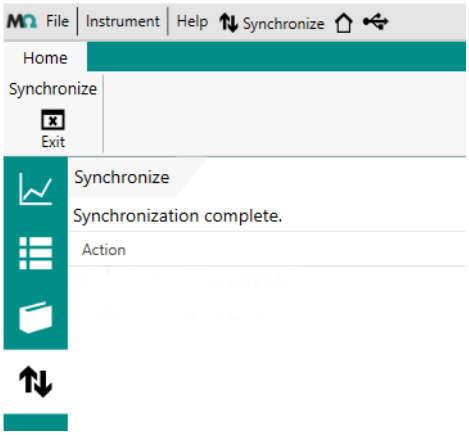


Operating Procedures	
Home ►	
Operating Procedures	List the operating procedure in the database. Click on an operating procedure to highlight and carry out actions. No actions can be taken on the default OP. Right click on a selected operating procedure to open a function menu.



Device Operating Procedures	List of operating procedures on the device. The user can add them to the database from the **Device Operating Procedures** section.
Reports	Generate a report for the selected operating procedures.

Synchronize view



The **Synchronize** view is only visible when **Auto Synchronize** is deactivated in the **Settings** *(see "Drop down menus", page 9)*.

Synchronize	
Synchronize	Opens the **Synchronize** view. Summarizes the synchronize actions. When the synchronization is complete, a window will open showing all operating procedures, user libraries and licensed libraries that are not in the database.
Home ▶	
Exit	Closes the **Synchronize** view.

3.5 Identification of samples with libraries

The measured spectrum of a substance is compared with existing spectra in a library that has been loaded to MIRA XTR DS / MIRA DS.

The **Illicit Library**, created by Metrohm Raman, is preinstalled on MIRA XTR DS / MIRA DS. Libraries can also be created by the user or purchased from commercial sources.

Creating a library

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

Purchase commercial libraries

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

Identification of a substance

Libraries are selected for matching when operating procedures are created.

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

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.

Processor	Multicore x86 processor (64-bit preferred)
Operating system	▪ Windows 10 (64-bit only) ▪ Windows 7 (Service Pack 3 or higher). In January 2020, Microsoft discontinued support for Windows 7. Support for Metrohm Raman software ended with the Microsoft lifecycle.
Screen resolution	Resolution 1024 x 768 or higher
RAM	All operating systems: 2 GB minimum; 4 GB recommended
Storage capacity	Minimum 100 GB; 500 GB recommended
USB connectors	USB 3.0
Mouse and keyboard	Required, USB, PS/2 style, or wireless
Keyboard	Compatible keyboard using USB / PS/2, or similar connection
System backup	Network or local backup required for data archiving.

NOTICE

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

4.2 Install MIRA Cal DS

NOTICE

Make sure to have administrator rights before installing MIRA Cal DS

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

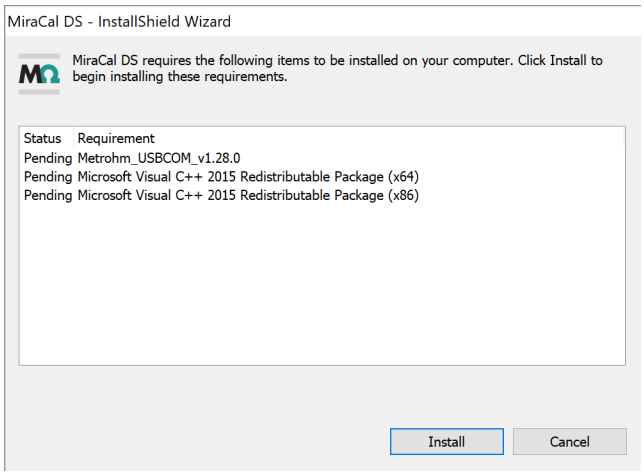
Installing the Metrohm USBCOM Driver

1 To download the latest version of MIRA Cal DS, click on the following link:

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

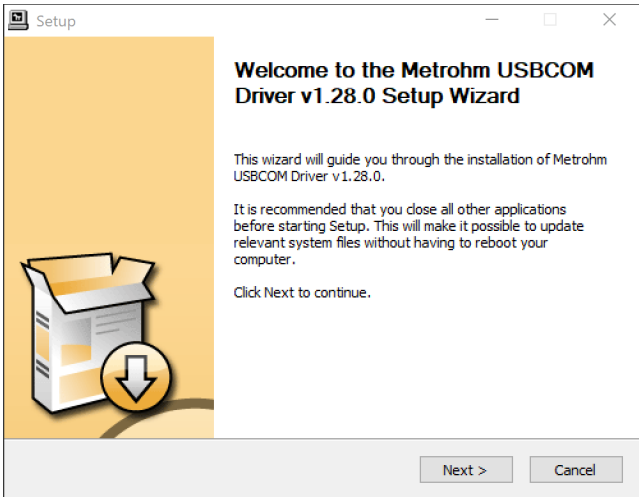
Double click on the installer.

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

3 

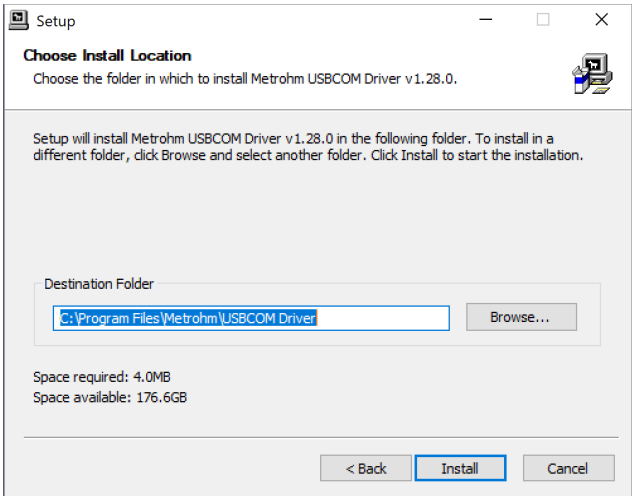
Click on **[Install]**.

4



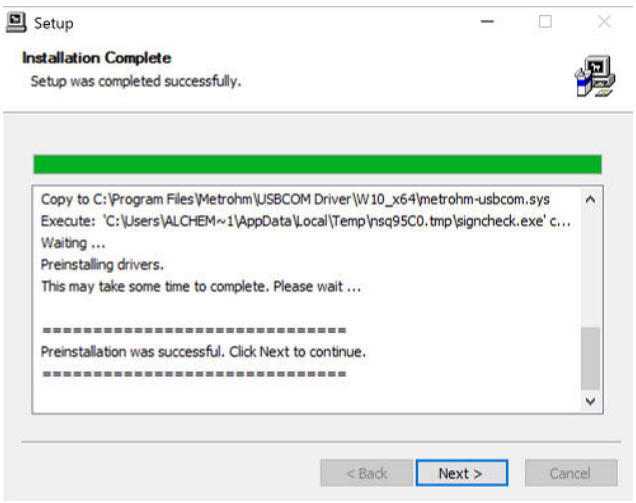
Click on **[Next]** to begin the installation of the driver.

5



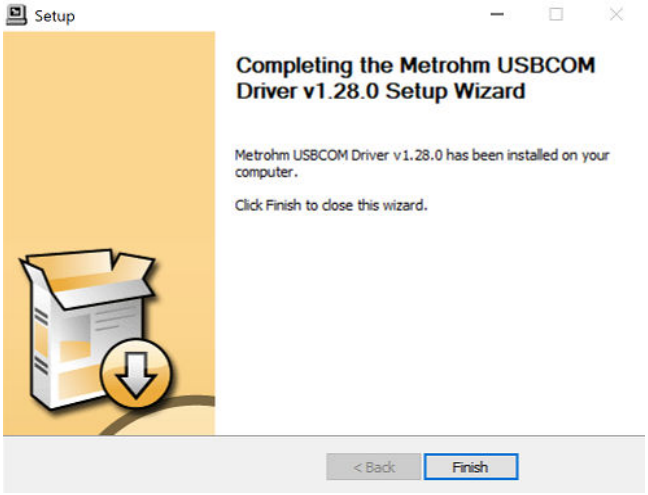
Click on **[Install]**.

6



Click on **[Next]**.

7



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

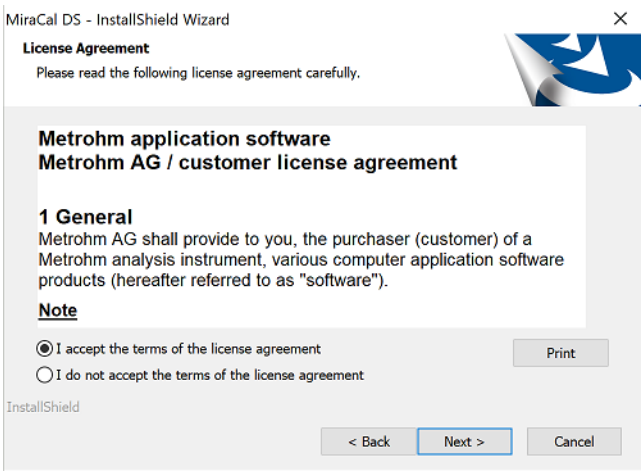
Installing MIRA Cal DS

After the installation of the Metrohm USBCOM Driver is completed, the MIRA Cal DS installation wizard starts automatically.

1

Click on **[Next]** to start the installation of MIRA Cal DS software.

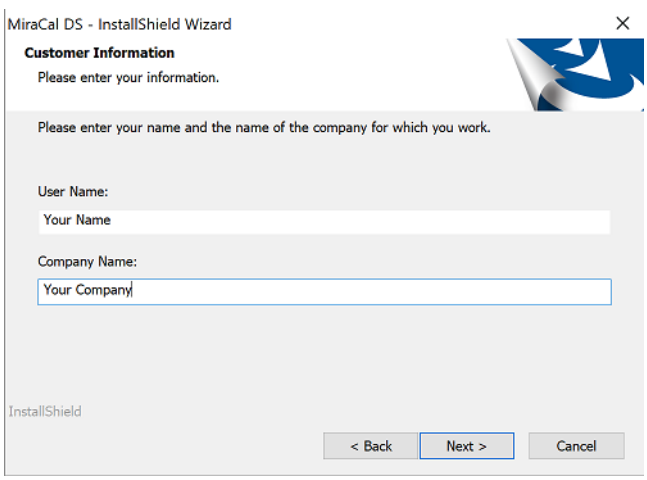
2



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

Click on **[Next]**.

3

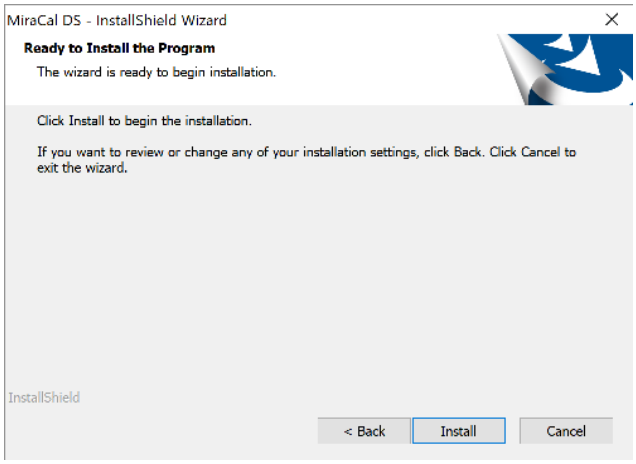


Enter your **User Name**.

Enter the **Company Name**.

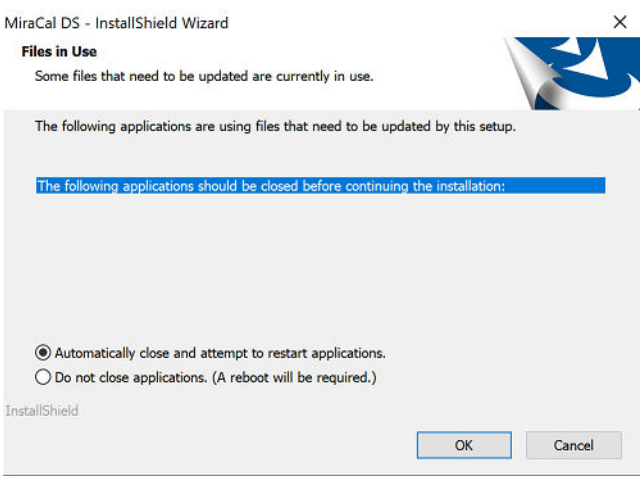
Click on **[Next]**.

4



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

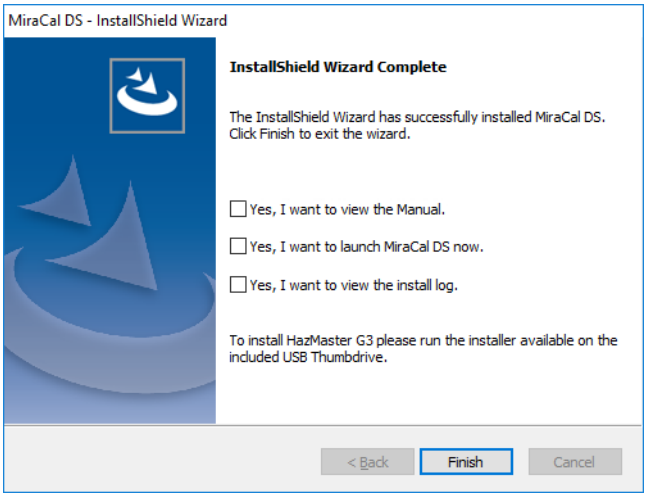
5



Select **Automatically close and attempt to restart applications.**.

Click on **[OK]**.

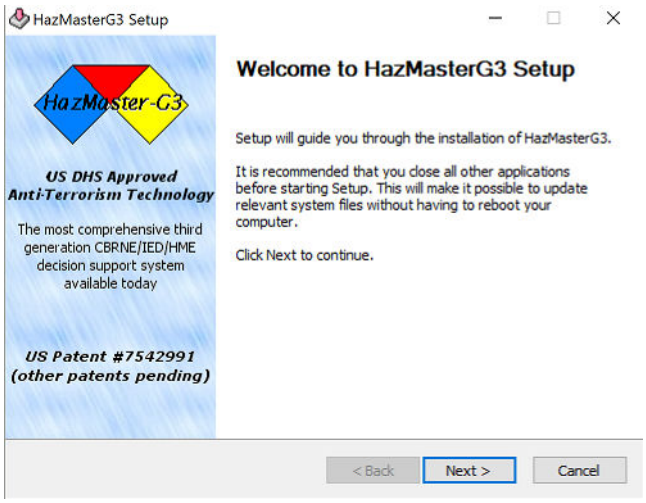
6



Click on **[Finish]** to complete MIRA Cal DS installation.

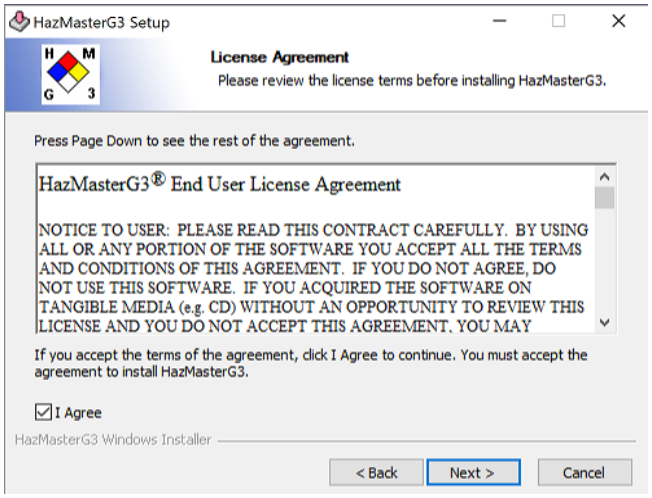
Installing HazMasterG3® software

1 If HazMasterG3 was purchased, copy the HazMasterG3 application from the USB drive and double click on the executable installation.



Click on **[Next]** to start the installation of HazMasterG3.

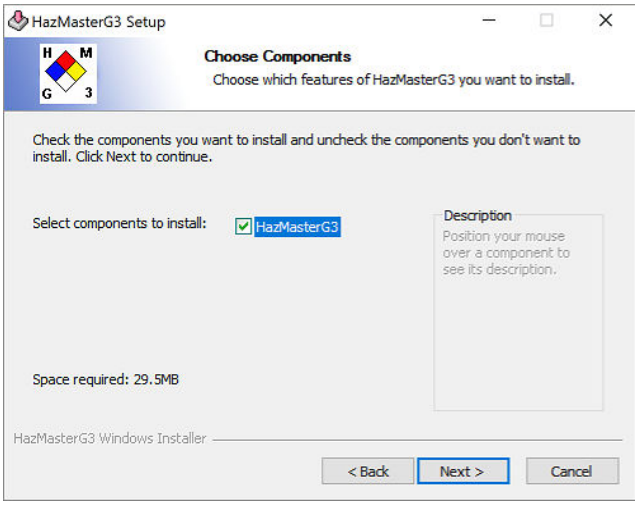
2



Check **I Agree**.

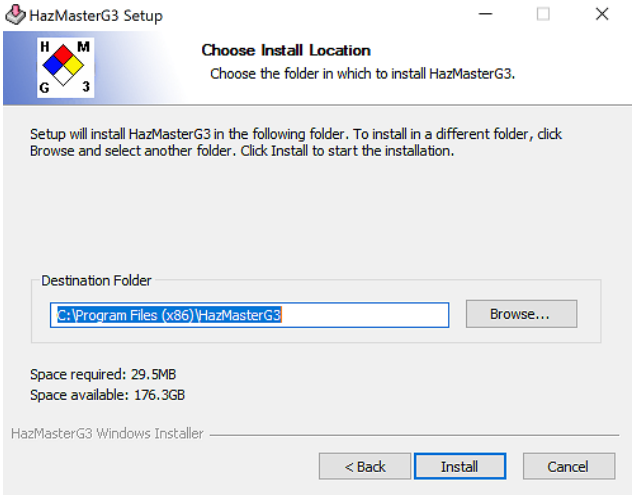
Click on **[Next]**.

3



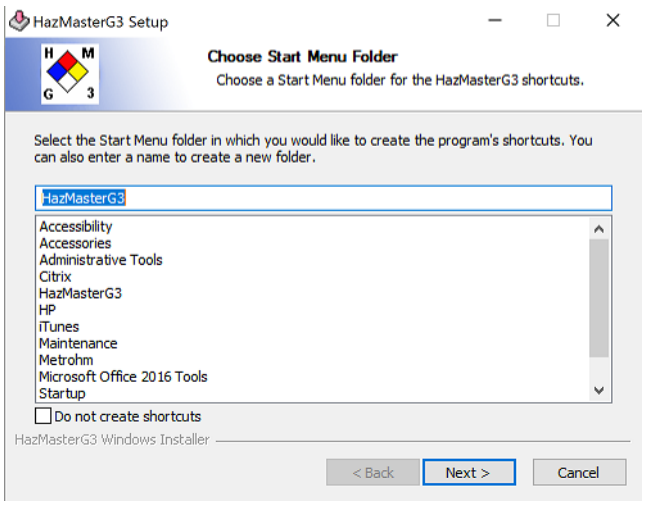
Click on **[Next]**.

4



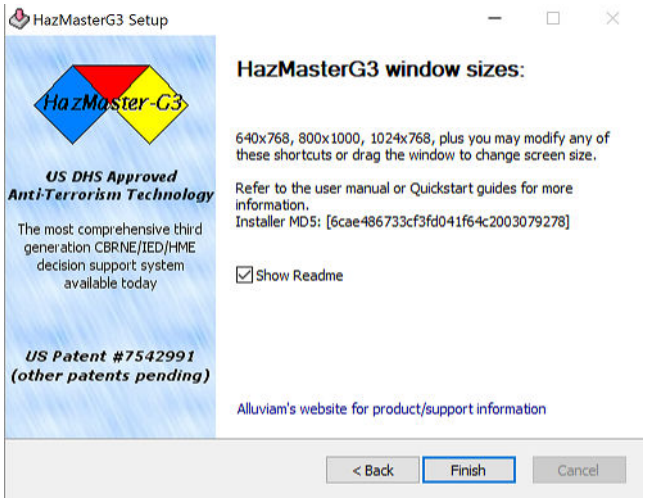
Click on **[Install]**.

5



Click on **[Next]**.

6



Click on **[Finish]** to complete HazMasterG3 installation.

5 Initial start-up

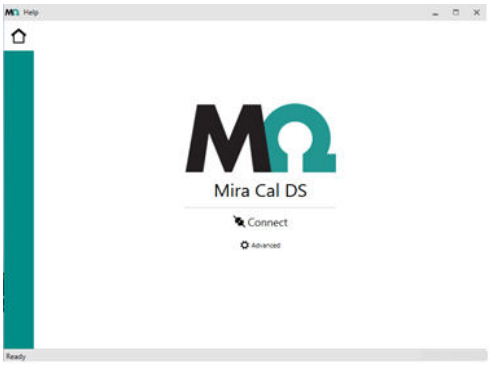
MIRA Cal DS is designed to operate as simply as possible. The software's main use is data synchronization and report generation. This is accomplished with simply connecting the instrument to the software. The data will automatically synchronize and reports will be generated. A sample summary report is the default but full report generation can be set as the default in the software setting tab.

5.1 Start MIRA Cal DS

1

Double click on the MIRA Cal DS icon on the desktop.

The home page for MIRA Cal DS opens.



5.2 Establish a connection between MIRA XTR DS / MIRA DS and MIRA Cal DS

NOTICE

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

Physically connect the instrument to the host computer

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

MIRA XTR DS / MIRA DS will automatically power on when connected to the host computer.

Wait a moment for the instrument to be ready. The PIN code screen displays.

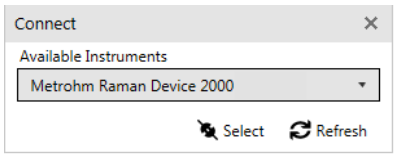
Enter the PIN code and wait until the Calibrate Device screen appears before connecting to the device.

Connect/Disconnect from the home page

1 On the home page of MIRA Cal DS, click on **[Connect]**.

The instrument will automatically connect and synchronize its data.

If more than one MIRA XTR DS / MIRA DS is connected, the user may be asked to select an available instrument.



Select **Metrohm Raman Device 2000** and click on **[Select]**.

After the initial connection of the MIRA XTR DS / MIRA DS, the software will recognize the instrument and not ask the user to select an available instrument.

NOTICE

If the instrument is not listed, make sure the instrument is turned on and booted to the **Calibrate Device** screen. The instrument will not be listed if it is turned off. Click on **[Refresh]**.

NOTICE

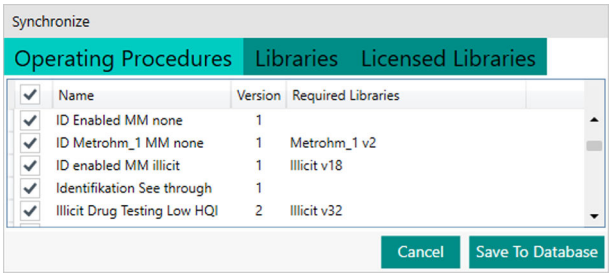
The icon in the menu bar of MIRA Cal DS indicates a successful connection.

The screen of the instrument displays **Connected**.

MIRA Cal DS will automatically synchronize when **[Connect]** is selected from the home page. MIRA Cal DS will inform the user.

✓ Synchronization Successful

2 If **Auto Synchronize** is turned off, device operating procedures, user libraries, and licensed libraries not in the database will be listed in the **Synchronize** view.



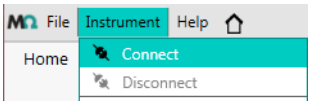
Click **[Save to Database]** to add selected items to MIRA Cal DS database.

3 To disconnect MIRA XTR DS / MIRA DS from the software, click on **[Disconnect]**.

Connect/Disconnect from advanced tools

1 On the home page of MIRA Cal DS click on **[Advanced]**.

2 In the menu tabs, select **Instrument ► Connect**.

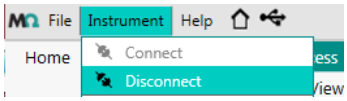


A synchronization progress window will appear showing the status of the actions being performed. When synchronization is complete, the bottom information bar displays **Ready**.

The MIRA Cal DS default is to automatically synchronize when you select **[Connect]**.

The user can change synchronization settings when MIRA XTR DS / MIRA DS is connected to the software.

3 To disconnect MIRA XTR DS / MIRA DS from the software, click on **Instrument ► Disconnect**.



NOTICE

More than 1 instrument can be used with the software. They can be synchronized to the same database in order to achieve a clean data management. However, the instruments cannot be connected to the software simultaneously, they must be used consecutively.

5.3 Configuration

5.3.1 Create and edit libraries

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

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

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

NOTICE

Use **Sample Browser** to find samples. The **Recent** tab allows the user to view recently viewed samples.

7 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.

8 Go to the **Library Samples** tab.

9 Double click on the library sample in the sample list and 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 MIRA XTR DS / MIRA DS identification screens.

10 Click on **[Save]** in the **Library Samples** tab to save sample meta data.

11 Click on **[Save]** in the **Library** tab to create the new library.

12 Check **Auto Synchronize** in the settings, to automatically synchronize new libraries, when you connect the MIRA XTR DS / MIRA DS instrument to the software.

If **Auto Synchronize** is deactivated, click **[Synchronize]** in the header to synchronize new libraries to MIRA XTR DS / MIRA DS.

Edit a library

1 Go to the **Library** view.

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

3 You can add and delete samples.

- To add a sample, go to the **Add Samples** tab. Select a sample. 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.
- To delete a sample, select a sample. Click on **[Delete]** in the **Library Samples** section of the **Home** tab.

4 Click on **[Save]**.

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

6 Library Sample Metadata can be edited in preexisting user libraries.

Remove a library

1 Go to the **Library** view.

2 Select a library from the list and click on **[Delete]**.

5.3.2 Create and edit operating procedures

Operating procedures direct the acquisitions and evaluations of spectra.

MIRA XTR DS / MIRA DS has **Smart Acquire**, a process that optimizes acquisition parameters to enhance sample evaluation. The default procedure on MIRA XTR DS / MIRA DS and in MIRA Cal DS automatically performs a smart acquire and evaluates spectra against all available libraries.

Users can create operating procedures that include smart acquire but limit the libraries used for evaluation.

Users can also design operating procedures that do not use smart acquire, but use the following acquisition options.

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

The following table shows all acquisition options for operating procedures.

Table 2 Acquisition options

Acquisition option	Description
Smart Acquire	Laser power, integration time, etc. are automatically adjusted depending on the type of sample used, environment and the amount of background lighting. This method is specifically useful when the user is unaware of the settings that should be used for an acquisition.
Laser Power (level)	The intensity of the laser can be reduced. Choose a value between 1-5. 5 is the maximum. The recommended value is 5. Reasons to lower the laser power are: ▪ Measuring critical materials such as explosive or flammable materials. ▪ Measuring materials with a low melting point. Liquid and solid forms of a compound have different spectra.
Auto Integration	The instrument automatically chooses the best Integration time for the current sample.
Integration Time (sec.)	The integration time indicates how long a single spectrum is recorded. The integration time is divided into two steps. ▪ Laser **ON** to acquire sample spectrum. ▪ Laser **OFF** to acquire reference. The actual time for a measurement is twice the entered value. The maximum integration time is 30 seconds.

Acquisition option	Description
Averages	If the value is higher than 1, the displayed spectrum is an average of multiple acquisitions. A higher value in this field will lead to a longer measurement time, because more spectra need to be acquired. The maximum number of averages is 30. Example: Enter **5** to have an averaged spectrum of 5 measured samples.
Scan delay	Enter a time into this field if the user intends to have a delay before a scan. Leave this field blank if the user does not intend to have a delay before a scan. The maximum scan delay is 59 minutes.
Smart Tip	Select the required attachment to measure your samples. If no dedicated smart tip is required, select **Allow all**.
XTR Mode	▪ **[Automatic]** automatically runs XTR processing if fluorescence is detected. ▪ **[Every Scan]** runs XTR on every scan even if fluorescence is not detected. ▪ **[Prompted]** prompts the user to process XTR if fluorescence is detected. ▪ **[Never]** never runs XTR processing.

Create an operating procedure

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

2 Go to the **Home** tab.

3 Click on **[New]**.

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

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

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

6 Go to the **Identification** tab. Select the library to be used for matching from the **Available Libraries**. 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]**.

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

The user can select the minimum Hit Qualitiy Index (HQI). The default value is 0.85.

The user can check **Enabled** to match against user enabled libraries on the instrument. This is useful if the instrument has a large number of targeted libraries installed. The user can activate a targeted sub-library instead of searching the entire large library.

7 Go to the **Mixture Identification** tab. Select the library to be used for mixture matching from the **Available Libraries**. Double click on the library or click on **[Add]** in the **Mixture Identification** section of the **Home** tab to move the library to **Mixture Identification Libraries**.

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

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

The user can check **Enabled** to mixture match against user enabled libraries on the instrument. This is useful if the instrument has a large number of targeted libraries installed. The user can activate a targeted sub-library instead of searching the entire large library.

8 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.

9 If you check **Auto Synchronize** in the settings, new operating procedures synchronize automatically when you connect the MIRA XTR DS / MIRA DS instrument to the MIRA Cal DS software.

If you do not check **Auto Synchronize**, it is necessary to click **[Synchronize]** in the header to synchronize new operating procedures to MIRA XTR DS / MIRA DS.

Edit an operating procedure

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

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

3 You can edit the following settings.

- **Metadata**
- **Acquisition**
- **Identification**
- **Mixture Identification**

4 Click on **[Save]**.

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

Remove an operating procedure

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

2 Select an operating procedure from the list and click on **[Delete]**.

5.4 Calibration and system suitability

Calibrate an instrument

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

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

Perform 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 an instrument.
2. Attach a Calibration Standard to the instrument.
3. Click on **Instrument ► System Suitability Test**.

   A dialog window 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 "Create support log file", page 54*).
4. Select a destination for the report file. Click on **[Save]**.

6 Operation and control

6.1 Data acquisition with MIRA XTR DS / MIRA DS

Acquire data

NOTICE

Refer to the device manuals for a detailed description of the following steps (*see "Additional information – Device manuals", page 2*).

1. If any changes were made, synchronize the instrument with MIRA Cal DS to upload operating procedures and user accounts.
2. Disconnect the instrument from MIRA Cal DS.
3. Calibrate if desired or skip calibration.
4. Go to the **Home** screen.
5. If preferred, change the operating procedure.
6. Acquire spectra.

Transfer acquired spectra from MIRA XTR DS / MIRA DS to MIRA Cal DS

1. Connect the MIRA XTR DS / MIRA DS instrument to the MIRA Cal DS software.
2. MIRA XTR DS / MIRA DS will synchronize to MIRA Cal DS either automatically or manually. This depends on your settings.

   If MIRA XTR DS / MIRA DS does not synchronize automatically, select **Instrument ► Synchronize** in the settings.

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

Data acquisition with MIRA XTR DS / MIRA DS connected to MIRA Cal DS

1 Connect the MIRA XTR DS / MIRA DS instrument to the MIRA Cal DS software.

2 Click on the **Acquire** tab.

3 Select parameters.

- Acquire
  - **Single Acquisition**
    Check no boxes.
  - **Continuous Acquisition**
    Acquisitions without clicking **[Acquire]**.
  - **Multi Acquisition**
    The user selects how many sequential acquisitions are done. The user selects the time interval between the sequential acquisitions.
- Acquisition settings
  If the **Operating Procedure Acquire** box is deactivated, the **Acquisition Settings** tab appears.
  - If you check no boxes, the user selects integration time, laser power and number of averages.
  - If you check **Auto Integration**, the process determines the integration time. The user selects the laser power and the number of averages.
  - If you check **Smart Acquire**, there are no user options for acquisition.
- Operating procedure
  The user can select operating procedures that are created in the software and stored on MIRA XTR DS / MIRA DS.
- **SERS Operating Procedure**
  This procedure only appears when the SERS Attachment is connected to the instrument and selected by the user for SERS detection.

4 Click on **[Acquire]**.

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

6.2 Displaying and managing data

6.2.1 Viewing a spectrum

When a spectrum is synchronized it is placed in the active viewing window. Double click on the spectrum name to view the matching results and the reference spectrum.

Filter

1. Click on the **Filter** tab. The user can filter large amounts of data by using the filter criteria.
2. Set the desired filter criteria to manage the viewing window data.
3. Click on **[Clear Filters]** to set the filters to default.

Spectral viewing window

1. Select a spectrum from the **Sample Browser**.
2. Choose between the following options. When unchecked the normal Raman spectrum will be displayed.
   - **[From Browser]**
   - **[Offset]** slightly offsets 2 overlaid spectra for easy comparison.
   - **[Baseline]** – Normal Raman data can be processed to remove a raised baseline for better viewing.
   - **[XTR]** displays the eXTRacted data collected with MIRA XTR DS.
   - **[Matches]** overlays the matches of the active spectrum in the viewing window.
   - **[Peaks]** labels the peaks in the spectral viewing window. Thresholds can be set to limit the number of peaks shown.
   - **[Normalize]** normalizes the tallest peak to 1 for comparing spectra with different intensities.
   - **[Legend]** shows a legend of the samples displayed in the spectral viewing window.

6.2.2 Sample list folder management

1. Select **Sample** view.
2. Folders can be created on the right side of the sample viewing window.

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

6.3 Processing a spectrum

Spectra can be processed or reprocessed by using different methods.

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

Identification

1 Select the library to match against from the **Library** drop down list.

2 Increase or decrease the number in **Matches** to define the number of results shown.

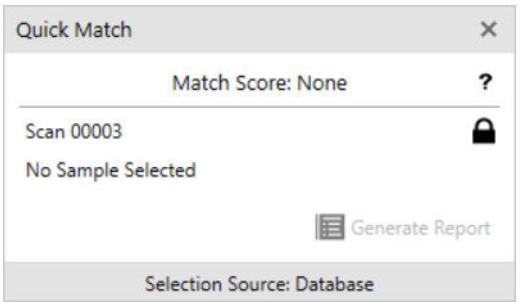
3 Increase or decrease the number in **Threshold** to define the threshold for the matching.

A higher threshold value increases the chances for false negatives. The default value is 0.85.

4 Click on **[Match]** to perform the match with the selected parameters.

Quick match

1 Select **[Quick Match]** to open the **Quick Match** window.

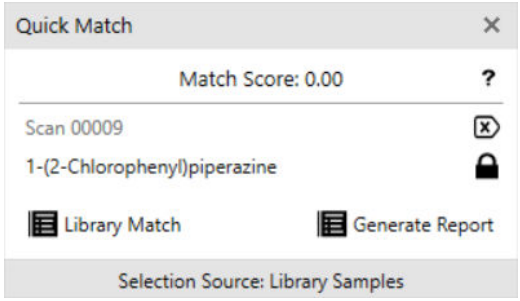


2 The selected spectrum will be shown. Press the icon to lock the active spectrum.

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.

Mixture identification

1 Select the library to match against from the **Library** drop down list.

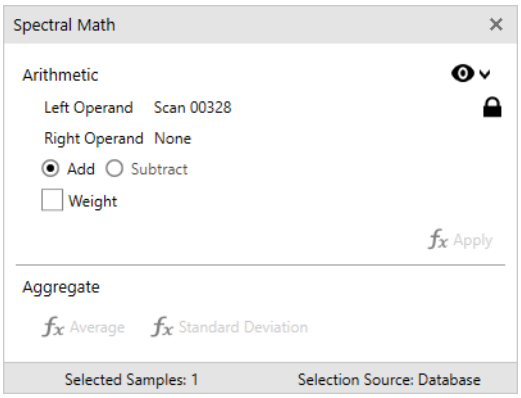
2 Increase or decrease the number in **Threshold** to define the threshold for the matching. A high number, for example 0.99, will increase the chances for forced matches. The default threshold is 0.920 for on device matching.

3 Click on **[Match]** to perform the mixture match with the selected parameters.

Spectral math

The user can perform basic spectral math on a spectrum. 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 Choose the operation 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 The result will be displayed in the active viewing window as a new spectrum.

To see a preview of the results, click on and activate **Preview Results**.

6.4 Generate 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 Select the **Sample** view.

2 Click on 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]**.

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 1

1. Select the **Libraries** view.
2. Click on 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 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]**.

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

Operating procedure report option 1

1. Select the **Operating Procedure** view.
2. Click on the **Reports** tab.
3. Click on **[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]**.

6.5 Export

Export samples

NOTICE

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

.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]**.

Export 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 .lrmp file type.

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

Export 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]**.

Export HazmasterG3 data

1 Go to the **Samples** view.

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

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

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

Export 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]**.

Save Baselined Data

1 Go to the **Samples** view.

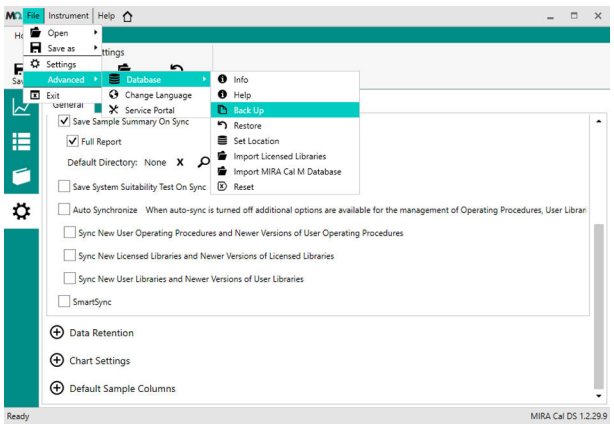
2 Select a sample. Activate **Baseline** to view baselined data in the viewing window.

3 Right click anywhere in the sample chart. Click on **[Save Raw Data]**.

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

6.6 Database backup

Exporting database

1 

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

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

Restoring database

NOTICE

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

An existing MIRA Cal DS database file must be available in **.litdb** format.

1. Click on **File ▶ Advanced ▶ Database ▶ Restore**.
2. Select the location of the database and the database file to restore. Click **[Open]**.
3. Confirm the restore. Select **[Yes]**.

6.7 Managing

6.7.1 Managing users

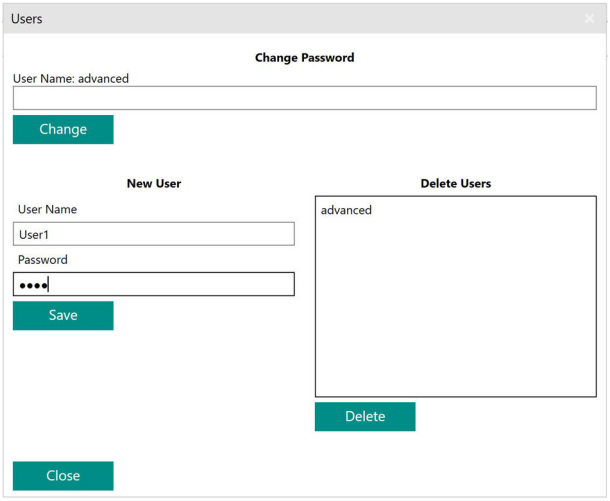


Figure 4 User management window

Activating the advanced login

1. To access the **Users** window, go to **File ▶ Settings**.
2. Check **Require Advanced Login**.
3. Change the password for the default advanced user by entering a password and click **[Change]**.

Creating and deleting users

1. Go to **File ▶ Settings**.
2. Click **[Manage Advanced Users]**.

3 Create a user name and password in the **New User** section and click **[Save]**.

4 Delete a user by selecting the user in the **Delete User** section and click **[Delete]**.

5 Click **[Close]** to close the **Users** window.

7 Create 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 should be attached to the instrument but is not necessary.

Instrument support log

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]**.