Brief Operating Instructions
Raman data library

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1   About this document

These instructions are Brief Operating Instructions. They are not a substitute for the Operating Instructions pertaining to the device.

1.1   Safety symbols

Structure of Information	Meaning
⚠ WARNING **Causes (/consequences)** Consequences of non-compliance (if applicable) ▸ Corrective action	This symbol alerts you to a dangerous situation. Failure to avoid the dangerous situation can result in a fatal or serious injury.
⚠ CAUTION **Causes (/consequences)** Consequences of non-compliance (if applicable) ▸ Corrective action	This symbol alerts you to a dangerous situation. Failure to avoid this situation can result in minor or more serious injuries.
NOTICE **Cause/situation** Consequences of non-compliance (if applicable) ▸ Action/note	This symbol alerts you to situations which may result in damage to property.

1.2   Safety

For information about the safe operation of Raman Rxn analyzers and the Raman RunTime Software, view the *Raman RunTime v6.5 Operating Instructions* (BA02180C). It is recommended that the *Raman RunTime v6.4* (or newer) *Operating Instructions* be read fully before using the Raman data library.

1.3   Documentation

All documentation is available:

- On the Endress+Hauser mobile app: www.endress.com/supporting-tools
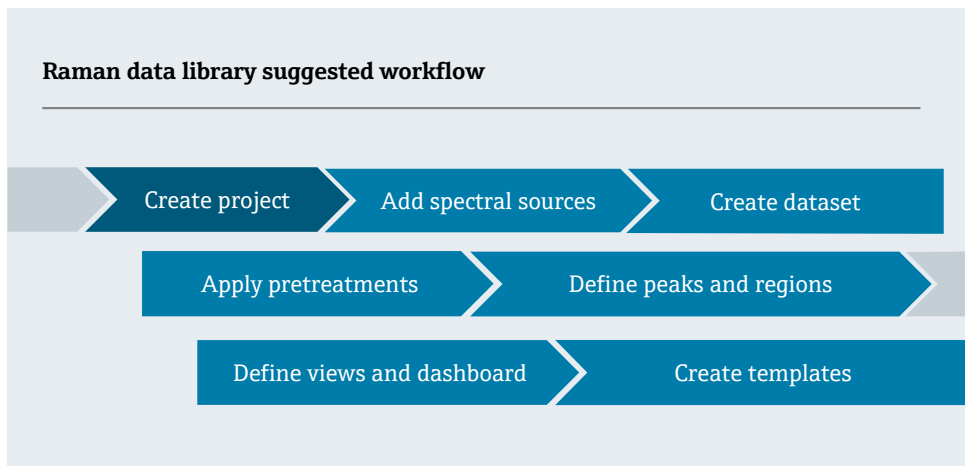- In the Downloads area of the Endress+Hauser website: www.endress.com/downloads

This document is an integral part of the document package, which includes:

Part Number	Document Type	Description
BA02367C	Raman data library User Operating Instructions	A complete overview of the software features and functionality for spectral data analysis.
BA02349C	Raman data library Administrator Operating Instructions	A complete overview of the operations related to managing security and the Raman data library database.

Part Number	Document Type	Description
TI01802C	Raman data library Technical Information	Planning aid for your data analysis system. The document contains all the technical data for the software.

2   Raman data library workflow

Raman data library has features and functions that can help build a workflow for spectral data analysis. A suggested workflow is shown below. Once you complete one portion of the workflow, such as importing data or applying pretreatments, the software opens the next step in processing your data.

Raman data library suggested workflow

Create project	Add spectral sources	Create dataset
Apply pretreatments	Define peaks and regions	
Define views and dashboard	Create templates	

2.1   Logging in (cGxP version only)

In the cGxP version, you must log in to open Raman data library. The login name and password are both required fields. The login name is not case sensitive. For example, the login name "Jane" is equivalent to the name "jane."

As a security precaution, if a user makes a configurable number of unsuccessful login attempts, they are automatically locked out. An administrator must be contacted to re-enable a locked-out user.

Use the following instructions to log into Raman data library for the first time.

1. After installation, confirm the Endress+Hauser Raman data library service is running in the list of Windows Services.
2. Double-click the Raman data library shortcut.

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Figure 1. Raman data library desktop icon

3. Log in to Raman data library with the first-time login information:

- The username is **Administrator**.
- The password is **Administrator1**.

You are required to change the password. Make note of the new administrator password.

When using system user authentication, create an additional user at this point. Adding one user in addition to the default administrator allows the administrator password to be reset if needed. Refer to *Creating a new user* in *Raman data library User Operating Instructions* (BA02367C).

2.2   Online and offline modes

Raman data library can be utilized from two different modes:
- **Online**. Live data from a Raman analyzer flows into the modeling software, offering real-time compositional analysis.
- **Offline**. Datasets are imported and can be analyzed independently of real-time processes. In offline mode, you can also create templates from known analytes, creating models and dataset templates to use and compare with real-time data.

Using these two modes enable you to understand and act upon the Raman spectra gathered in real-time process environments.

2.3   User interface

When launching Raman data library for the first time, a blank dashboard displays with left-side menu icons. Raman data library opens to a blank dashboard until a dataset is loaded and views are configured.

To ensure the intended UI experience within Raman data library, set your display scaling to 100 %.

2.3.1   Menus

Main menu

The main menu on the left side of Raman data library provides navigation between functions of the software.

Menu item	Navigation
≡ A0055967	**Expand/collapse**. Show or hide the menu items.
⬚ A0055968	**Dashboard.** Create and manage user dashboards.
⬚ A0055969	**Datasets.** Create and manage datasets.
⬚ A0055970	**Analyze Dataset.** Analyze the active dataset. Only enabled when there is an active dataset. This item contains five sub-tabs:

Menu item	Navigation
	▪ Data ▪ Pretreat ▪ Peaks/Regions ▪ Views ▪ Summary
![A0055971]	**Data Fields.** Create and manage data fields.
![A0055972]	**Spectral sources**. Create and manage spectral sources (OPC/SPC).
![A0055973]	**Projects**. Create and manage projects.
![A0055974]	**Users.** Create and manage users.
![A0055975]	**Settings.** Manage system settings.

Ribbon toolbar

The top of the Raman data library contains a ribbon toolbar. From the ribbon toolbar, you can:

- **Select a project.** The Selected Project list on the top menu bar allows you to switch between projects. For information about projects, refer to *Projects* → 🖹.

- **Change user (cGxP version only).** Clicking this tool allows you to switch to a different user while keeping the program running. To log out of the current user or session, exit the software by clicking the **X** button in the top right corner.

  For descriptions on changing users and passwords, see *User management* in the *Raman data library User Operating Instructions* (BA02367C).

- **Change password (cGxP version only).** Clicking this tool allows you to change your password.

- **About**. Clicking this tool displays the software version, version number, installation ID, and copyright information.

Figure 2. Ribbon toolbar

For information about projects, refer to *Projects* in the *Raman data library User Operating Instructions* (BA02367C). For descriptions on changing users and passwords, see *Users and Security* in the *Raman data library User Operating Instructions*.

3 How to start

After you install Raman data library, you must bring data into the software. This chapter outlines start-up tasks to get Raman data library ready for first-time use.

3.1 Importing Raman spectra and creating datasets

This section describes a quick-start approach to getting data into Raman data library. This is done by creating a dataset and navigating to a folder of spectra.

Saving your first dataset can take a few minutes. Subsequent saves are faster.

To create a dataset

1. Select **Datasets** from the menu.

   The **Existing Datasets** page displays.

2. Click **Create New Dataset**.

3. Enter a name for the dataset.

4. In the **Data Source** list, select **Imported Spectra**.

5. Browse to the folder with spectra files, then click **Select Folder**.

   When the import is complete, a folder and list of spectra appears. By default, all spectra are selected. Shift, Ctrl, and Ctrl+A can be used to choose specific spectra.

6. Leave all spectra selected or select the desired spectra. Click **Include**.

   Spectra included in the new dataset are shown under **Included Spectra**.

7. Check a box to include all spectra from the selection in Step 6 or include only a subset of the selection in which the software selects every second or third spectra.

8. Click **Create**.

   When the dataset is complete, the **Analyze Dataset** screen displays.

9. Click **Save Dataset**.

   A date and time appear after **Last Saved**.

10. Analyze and pretreat the data in the **Analyze Dataset** window. You can also resize plots and sections to customize views, and mark Accumulations and Exposure Length as displayed in the Data Fields list.

11. Click **Launch Dashboard** to view the dashboard for your new dataset.

From the dashboard, you can add new dashboard tabs, copy dashboards, and modify dashboards. Continue the Raman data library workflow by adding spectral sources, analyzing data, applying pretreatments, and controlling your Raman analyzer. Refer to *Raman data library User Operating Instructions* (BA02367C) for instructions.

3.2   Spectral sources

Spectral sources are sources of spectral data. A spectral source can be a watched input folder containing spectroscopic files (.spc) or spectra transferred in real time through an OPC connection to a Raman Rxn analyzer. In the cGxP version of Raman data library, the Spectral Sources Manager role is required to add or make changes to Spectral sources.
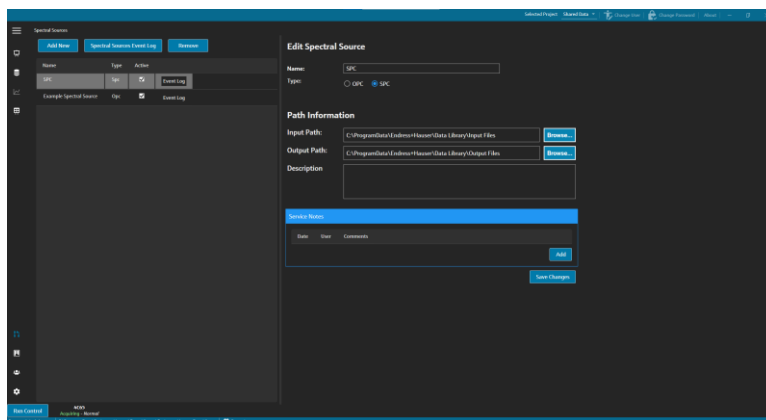

Figure 3. Spectral sources window

3.2.1   Adding an OPC spectral source

An OPC spectral source can be created to allow Raman data library to make an OPC unified automation (UA) client connection to a Raman RunTime OPC server. The OPC connection allows users to view, control, and collect spectra from Endress+Hauser Raman Rxn analyzer systems. Multiple Raman analyzers (up to 4) can be connected to Raman data library.

A minimum of Raman RunTime v6.4 is required for an OPC connection between Raman data library and Raman RunTime. Raman Rxn analyzers running Raman RunTime versions lower than v6.4 can use an SPC spectral source as described in *Adding an SPC spectral source* →🖺.

When an OPC spectral source is used, disable the device sleep feature in Windows settings.

To add an OPC spectral source

1. From the Spectral sources window, click **Add New**.
   The Edit Spectral source pane displays.

Figure 4. Edit OPC spectral source

2. Enter a name for the spectral source.
3. Select **OPC**.
4. Enter the following connection settings information:

    - **Host Name**. The host name or IP address of the Raman RunTime OPC server.
    - **Username**. The username used for creating the OPC connection to the Raman RunTime OPC server. Default: "kaiser-opc".
    - **Password**. The password used for creating the OPC connection to the Raman RunTime OPC server. Default: "opc".
    - **Description**. An optional description of the OPC spectral source.
    - **Status**. A status of the OPC spectral source, either Active or Inactive.
    - **Service Notes**. Service personnel or user comments about the OPC spectral source. Click the **Add** button to add a new service note.

5. Click **Test Connection** to check the connection to the Raman RunTime OPC server. To ensure a successful connection:

    - Perform a test connection before saving an OPC spectral source.
    - If using the host name of the analyzer does not result in a successful connection, try using the IP address. This may simply be due to host name resolution not configured correctly on your local IT/OT network.
    - As an alternate to the default OPC credentials, you can also use credentials for one of the user accounts configured on the Raman RunTime analyzer to authenticate the analyzer OPC connection.

6. Click **Save Changes**.

If the connection is successful, a message displays and the Rxn Control toolbar appears on the bottom ribbon, showing the assigned spectral source name and its status.

3.2.2   Adding an SPC spectral source

The SPC spectral source feature automatically imports spectra from Raman Rxn analyzers running Raman RunTime versions lower than v6.4. This enables the use of Raman data library with Endress+Hauser's legacy Raman software solutions. Adding an SPC spectral source allows Raman data library to automatically read and store .spc files within the Raman data library database and make them available for datasets.
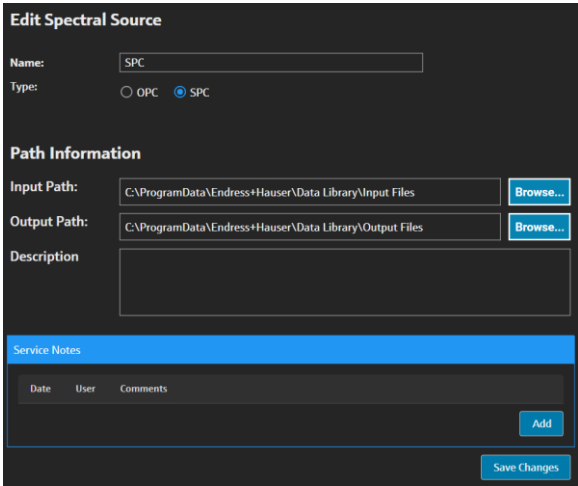
The SPC spectral source requires an input path, in which Raman data library watches for new files and imports them, and an output path, to which Raman data library moves the SPC files after they are imported.

Refer to *SPC file network export* in the *Raman RunTime Operating Instructions* (BA02180C) for instructions on exporting .spc files from Raman RunTime.

To add an SPC spectral source

1. On the Raman data library computer, create .spc folder(s):
    - For Raman RunTime versions lower than v6.4, create one folder named **Output spectra**.
    - For legacy software solutions, create two folders. Name one **Input spectra**, and the other **Output spectra**. Configure the legacy software to output .spc files to the **Input** folder.

2. Click **Spectral sources** 🎚, then click **Add New**.

    The Edit Spectral source pane displays.

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Figure 5. Edit SPC spectral source

3. Enter a name for the spectral source.
4. Select **SPC**.

5. In **Input Path**:
   - For Raman RunTime versions lower than v6.4, browse to the network shared folder at the path *computer name or IP address*\DataLibraryBatchExport.
   - For legacy software solutions, point the **Input path** to the legacy software's output directory.
6. In **Output Path**, browse to the output spectra folder created in Step 1. This is the directory path used for outputting .spc files after they have been read into the system.
7. (Optional) Enter the following information:
   - **Description**. A description of the SPC spectral source.
   - **Service Notes**. User comments about the SPC spectral source. Click the **Add** button to add a new service note.
8. Click **Save Changes** and **OK** to the prompt.

In Raman RunTime versions lower than v6.4, the network shared DataLibraryBatchExport folder contains subfolders and .spc files acquired on the Raman analyzer. Once the .spc files have been read and added to Raman data library, the files are moved from this network directory to the Output spectra folder created above. All .spc files are retained on the Raman analyzer. The files are only moved out of the DataLibraryBatchExport folder.

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