# User Operating Instructions
# Raman data library 2.0



Endress+Hauser

People for Process Automation

# Table of Contents

# 1     About this document

## 1.1     Document function

This document gives instructions related to general user tasks for Raman data library including navigation, field explanation, data manipulation, and more. For administrative instructions including installation, database and user management, and security, refer to the *Raman data library Administrator Operating Instructions* (BA02349C).

## 1.2     Safety symbols

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

## 1.3     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.

### 1.3.1     IT safety

IT security measures, which provide additional protection for the device and associated data transfer, must be implemented by the operators in line with their security standards.

## 1.4     Glossary

| Term | Description |
|---|---|
| Audit Trail | Independent computer-generated record of changes to electronic records indicating time, operator, action, content and if needed, reason. |
| Authorized User | End user who has completed the required training and been granted access to the application. |
| BCA | Background Correction Accuracy |
| ˚C | Degrees Celsius |
| Cfm | Cubic feet per minute |
| CFL | The new CFL file format defined in "Galactic Industries Corp. Universal Data Format Specification", dated September 4, 1997 |
| CFR | Code of federal regulation |
| cGMP | Current good manufacturing practices |

| Term | Description |
|------|-------------|
| cGxP | Current good clinical, laboratory, and/or manufacturing practices |
| CMMS | Computerized maintenance management system: a computer-based database that contains all of the maintenance work orders and is utilized for scheduling activities. |
| COTS | Configurable off–the-shelf |
| CTQ | Critical to quality |
| Critical requirement | A requirement that, if not met, has an adverse impact on any of the regulatory agency requirements, data integrity or security. |
| Data Analysis | Any work process with the goal of obtaining useful information from the raw data supplied by the spectrometer. |
| Electronic Record | Any combination of records represented in digital form that is created, modified, maintained, archived, retrieved, or distributed by a computer system and used for a cGxP regulated activity. |
| Electronic Signature | Authorization of the electronic record by an individual in the form of digital confirmation that is legally binding and equivalent to the individual's handwritten signature. |
| Final Report | A document summarizing all results derived from the execution of a validation document. |
| GAML | Generalized analytical markup language |
| GDP | Good documentation practices |
| GCC | Global change control |
| GHz | Gigahertz |
| Graphical Data | Key data, information, attributes that can be represented in a graphical format. |
| Hz | Hertz |
| IAPP | Information asset protection policy |
| In Situ | In its original place |
| IQ | Installation qualification |
| LAN | Local area network |
| Nm | nanometers |
| Non-Critical requirement | A requirement that, if not met, does not have an adverse impact on any of the regulatory agency requirements, data integrity or security. |
| OQ | Operational qualification |
| OS | Operating system |
| Password | The unique, private code input by the user for identification purposes. |
| PAT | Process analytical technology |
| PC | Personal computer |
| ppb | Parts per billion |
| ppm | Parts per million |
| psig | pounds per square inch gage |
| Savitzky-Golay filter | A digital filter that can be applied to a set of digital data points for the purpose of smoothing the data, that is, to increase the precision of the data without distorting the signal tendency. |
| SPC | File form defined by developer. |
| Spectra | The raw data from the Raman spectrometer after processing into SPC (GRAMS) format. |
| QC | Quality control |

| Term | Description |
|---|---|
| Raman Rxn4 analyzer | An integrated spectroscopy system designed to accommodate fiber optic probes for the purpose of sample analysis. |
| RAM | Random access memory |
| UPS | Uninterruptable power supply |
| URS | User requirements specification |

## 1.5    Documentation

All documentation is available:

- On the media device supplied (not included in the delivery for all device versions)
- 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 |
|---|---|---|
| BA02349C | Raman data library Administrator Operating Instructions | A complete overview of the operations related to managing security and the Raman data library database. |
| KA01717C | Raman data library Brief Operating Instructions | A quick start guide for running Raman data library after installation. |
| TI01802C | Raman data library Technical Information | Planning aid for your data analysis system. The document contains all the technical data for the software. |

## 1.6    Registered trademarks

**SIMCA®**
Registered trademark of Sartorius Stedim Biotech.

**GRAMS IQ™**
Registered trademark of Thermo Fisher Scientific.

# 2 Product description

Endress+Hauser's Raman data library is a software program designed to organize, visualize, analyze, and report on Raman Rxn spectral data. Raman data library complements the Endress+Hauser Raman Rxn embedded Raman RunTime by providing spectra storage, organization, analysis, and multi-analyzer data collection from lab to cGxP.

Raman data library was created for users who need to visualize Raman spectra, associate it with reference data, and create univariate peak models. With this software, prepared data can be exported for external multivariate modeling.

Raman data library features:

- **Data organization.** Matches spectra to reference values, prepares data prior to chemometric modeling, provides searchable data storage, and ensures data integrity.
- **Data analysis**. Gives enhanced spectra visualization and simple analysis such as peak trending and univariate modeling.
- **cGxP option**. Meets industry standards for spectral data traceability, storage, and archival.

Raman data library stores spectral data in a secure, embedded SQLite database, performs calculations on the spectral data, and displays spectral data and its associated metadata in reports and on-screen. This functionality allows Raman spectra to act as reference data for quantitative Raman method development and support the needs of FDA 21 CFR part 11 as part of a validated analytical solution.

Raman data library can be implemented to be 21 CFR part 11 compliant when installed with the cGxP Setup installer and qualified through IQ/OQ with Endress+Hauser, and PQ with the customer. When installed in cGxP mode, the program facilitates collection, storage, and organization of Raman spectra so that spectra may:

- Act as calibration set data for quantitative Raman model development as part of a validated analytical solution, or
- Act as data input into validated models used for predictions of process or sample properties

## 2.1 Installation

Raman data library is designed to be installed on a standalone workstation. Raman data library contains functionality to export data from each instance of the application and import the data into a centralized location. Refer to the installation instructions in the *Raman data library Administrator's Operating Instructions* (BA02349C).

## 2.2 Security settings (cGxP version only)

In cGxP environments, Raman data library utilizes user authentication to ensure traceability and logging of all events. In Raman data library core environments, user management and authentication are not utilized.

From the Settings window, you can modify system security settings. To make changes to system security settings, you must be logged in with a System Settings Manager role.
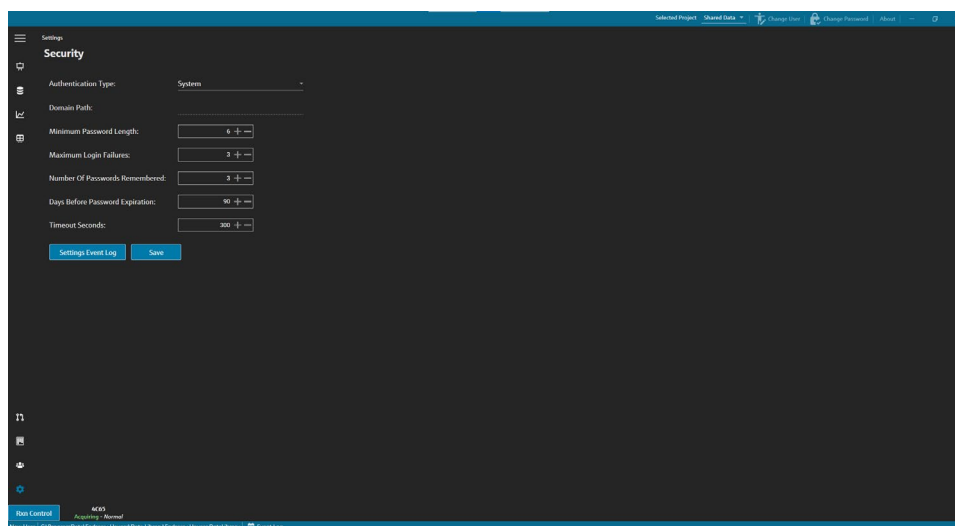


*Figure 1. Security window*

From the Settings window, you can select:

- **Authentication type.** The authentication type for the application. The user can choose between System, Domain, and Local authentication modes.
- **Domain path.** (Domain authentication only) The domain path.
- **Minimum password length.** The minimum number of characters for a user password. The minimum number of characters allowed is 6.
- **Maximum login failures.** The number of failed log-in attempts that are allowed before a user account is locked out.
- **Number of passwords remembered.** The number of unique new passwords that must be associated with a user account before an old password can be reused.
- **Days before password expiration.** The period of time (in days) that a password can be used before the system requires the user to change it. You can set passwords to expire after a certain number of days or you can specify that passwords never expire by setting the number of days to 0.
- **Timeout seconds.** The period of time (in seconds) of allowed inactivity before a system timeout occurs. After a system timeout, users are required to reenter credentials to continue or exit the application. If the Timeout Seconds is set to 0, the system timeout is disabled. The max configurable timeout value is 3600 seconds (60 mins).
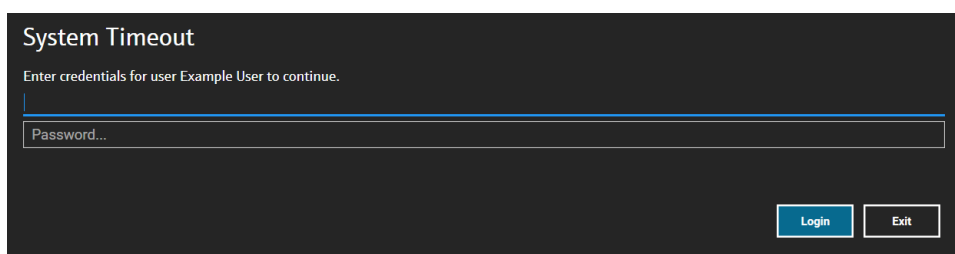


*Figure 2. System timeout*

- **Save.** Saves the system security settings.
- **Settings event log.** Displays the event log for settings.

## 2.3     User management (cGxP version only)

In cGxP environments, Raman data library authenticates users to ensure traceability and logging of all events. The core version of Raman data library does not offer user management and authentication.

The Users window allows managers to add, update and delete user accounts. It also allows managers to view events by a specified user or all events by all users. To manage users, you must be logged in to an account with the Users Manager role.
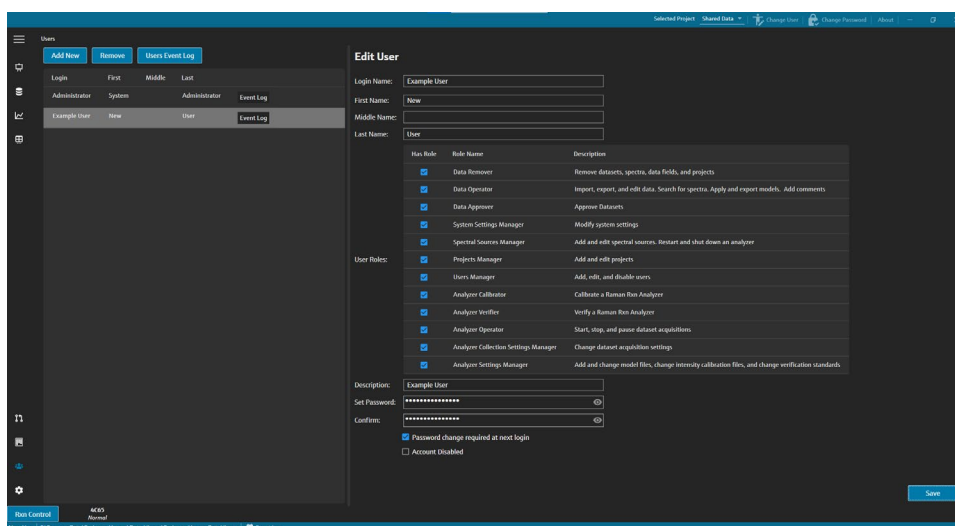


*Figure 3. Users window*

From the Users window, you can select:

- **Add New.** Creates a new user.
- **Remove.** Removes the selected user. The Data Remover role is required to remove a user.
- **Users Event Log.** Displays the event log for all users.
- **Event Log.** Displays the event log for the specified user.

## 2.3.1 User roles

Within the user roles functionality, a user manager can create users with privileges that follow the organizational structure determined by the customer. As such, fixed user groups are not present. Instead, there are many options for structuring privileges by assigning a combination of user roles.

User roles can be utilized to limit user functionality. Any combination of roles may be assigned to a given user, from all roles to no roles.

| Role | Actions allowed |
|---|---|
| Data Remover | <ul><li>Remove datasets</li><li>Remove spectra</li><li>Remove data fields</li><li>Remove projects</li></ul> |
| Data Operator | <ul><li>Import, export, and edit data</li><li>Search for spectra</li><li>Apply and export models</li><li>Add comments</li></ul> |
| Data Approver | Approve datasets |
| System Settings Manager | Modify system settings |
| Spectral Sources Manager | <ul><li>Add and edit spectral sources</li><li>Restart and shut down an analyzer</li></ul> |
| Projects Manager | <ul><li>Add projects</li><li>Edit projects</li></ul> |
| Users Manager | <ul><li>Add users</li><li>Edit users</li><li>Disable users</li></ul> |
| Analyzer Calibrator | Calibrate a Raman Rxn analyzer |
| Analyzer Verifier | Verify a Raman Rxn analyzer |
| Analyzer Operator | <ul><li>Start dataset acquisitions</li><li>Stop dataset acquisitions</li><li>Pause dataset acquisitions</li></ul> |
| Analyzer Collection Settings Manager | Change dataset acquisition settings |
| Analyzer Settings Manager | <ul><li>Add and change model files</li><li>Change intensity calibration files</li><li>Change verification standards</li></ul> |

User roles can be restricted to one set of privileges or combined into sets related to a functional role's responsibilities. The following table gives examples of role sets that could be assigned to users, supervisors, and administrators.

| User Level | Roles applied |
|---|---|
| User | ▪ Data Operator<br>▪ Spectral Sources Manager<br>▪ Analyzer Calibrator<br>▪ Analyzer Verifier<br>▪ Analyzer Operator<br>▪ Analyzer Collection Settings Manager<br>▪ Analyzer Settings Manager |
| Supervisor | ▪ Data Remover<br>▪ Data Approver<br>▪ System Settings Manager<br>▪ Projects Manager |
| Administrator | ▪ Users Manager |

## 2.3.2    Creating a new user

**To create a new user**

1.   From the Users window, click **Add New**.

     Create new Raman data library user accounts for all new system users.  While Raman data library can rename users, only use this functionality to upgrade a user's name because of a name change. Do not rename a user account to reassign the account to a new individual.

     A new Edit User pane displays.



*Figure 4. Edit User pane*

2.   Enter the user properties:

     ▪   **Login Name**. The name used to login to the system. Each login name must be unique and from 1 to 100 characters in length.

     ▪   **First Nam**e. The user's first name.  It may be from 0 to 100 characters in length.

     ▪   **Middle Name**. The user's middle name.  It may be from 0 to 100 characters in length.

     ▪   **Last Name**. The user's last name.  It may be from 0 to 100 characters in length.

     ▪   **User Roles**. The roles the user is granted in Raman data library.  User roles can be added or removed by selecting or deselecting the **Include** checkbox for each role. See *User roles →* 📄.

     ▪   **Description**. A description of the user.

3.  Enter a valid password in the **Set Password** and **Confirm Password** boxes.

    A password must meet the following minimum password requirements:

    - Must contain at least one special character
    - Must contain a mixture of uppercase and lowercase letters
    - Must meet the minimum password length which is set on the Settings window

4.  (Optional) Select **Password change required at next login** when adding a new user.
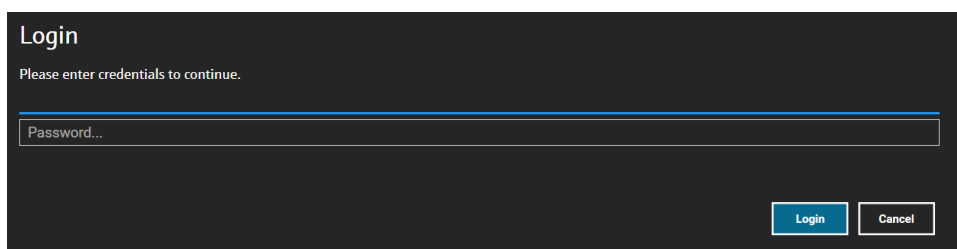
5.  Click **Save**.

### 2.3.3  Disabling a user

Inactive Raman data library user accounts can be disabled but should always be retained in Raman data library for historical and audit trail purposes. A disabled user may not login.

**To disable a user**

1.  From the Users window, select the user account to disable.

2.  Select **Account Disabled**.

3.  Click **Save**.

### 2.3.4  Changing the user

Click **Change User** on the top ribbon toolbar to switch to a different user. User credentials must be entered correctly to switch to a different user.



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*Figure 5.User login*

### 2.3.5  Changing the password

Click **Change Password** on the top ribbon toolbar to change the password for the current user. The user is required to enter the old password, the new password, and then confirm the new password.

The password must meet the minimum password requirements. A password must contain at least one special character, a mixture of uppercase and lowercase letters, and meet the minimum password length, which is set on the Settings window.
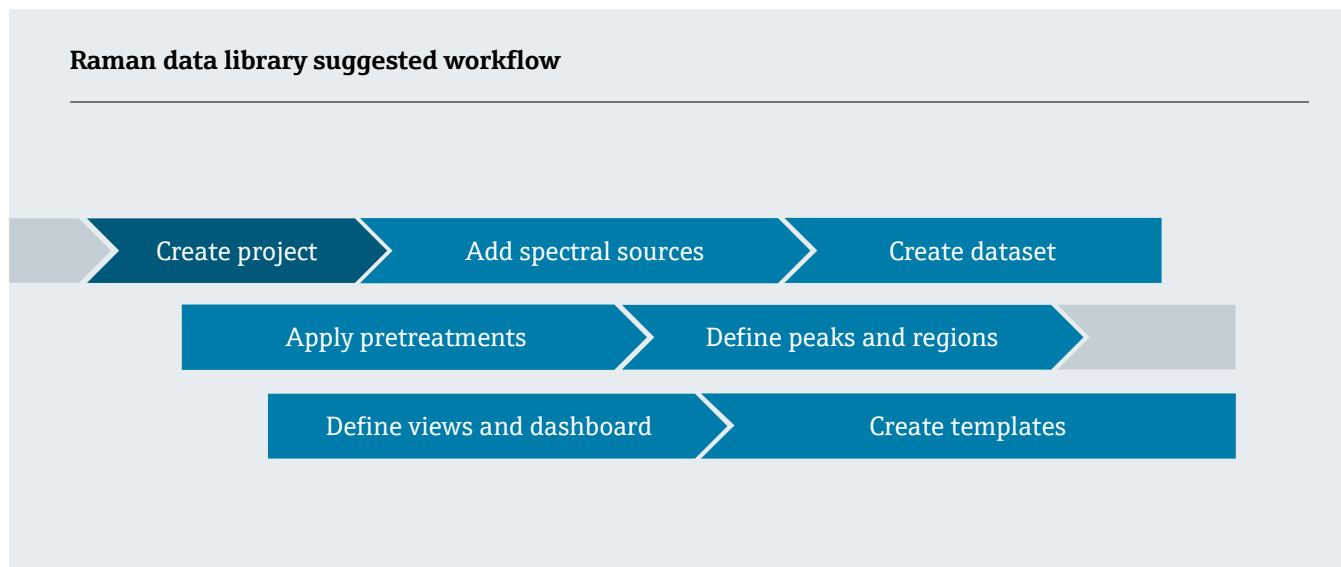


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*Figure 6. Change Password dialog*

This menu item is not available if the authentication mode is set to Local Windows or Domain. With these authentication modes, password changes are handled by the selected authentication server.

# 3      Software operation

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

This manual is designed to follow that workflow, moving from adding data to Raman data library to creating projects, using pretreatments, and analyzing data.

After you install Raman data library, you must familiarize yourself with the software interface to develop a data analysis workflow that suits your needs. Refer to the *Raman data library Brief Operating Instructions* (KA01717C) for quick start instructions.

## 3.1      Logging in (cGxP version only)

In the Raman data library 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.

## 3.2      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**. Data sets are imported and can be analyzed independently of real-time process. 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.

## 3.3      User interface

When launching Raman data library for the first time, a blank dashboard displays with left-side menu icons. The left menu can be expanded. 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 Windows display scaling to 100 %.

### 3.3.1    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:<br>▪ Data<br>▪ Pretreat<br>▪ Peaks/Regions<br>▪ Views<br>▪ 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. This feature is available to the cGxP version of Raman data library only. |
| A0055975 | **Settings**. Manage system settings. This feature is available to the cGxP version of Raman data library only. |

**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. For descriptions on changing users and passwords, see *User management (cGxP version only)*.
- **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 7. Ribbon toolbar*

### 3.3.2    Data library dashboard

The dashboard is the main view for routine analysis. It displays tabs that can be configured to show plots of saved datasets. A dashboard tab can contain views from more than one dataset. One or more datasets must be defined to display views on the dashboard.

To use the dashboard, you must first follow an initial setup outlined at the beginning of this chapter and described in *Adding data to Raman data library* → 🖺 and *Analyzing datasets* → 🖺. You can also refer to the *Raman data library Brief Operating Instructions* (KA01717C) for a quick start guide.

When Raman data library is launched, dashboard tabs from the previous session are loaded. If no previous dashboard has been defined, as during first use of the software, the dashboard is blank. Previously saved dashboard tabs can be reloaded by clicking **Launch Dashboard** from the Summary tab of the Analyze Dataset window. Dashboard tabs are automatically saved when Raman data library is closed.

When the dashboard is configured and launched for a new dataset, it provides two default views: the spectra grid and spectra plot. Additional views for a dataset are defined from within analyze dataset, under the **Views** tab. Refer to *Creating dashboard views: grids, trends, spectra, and 3D plots →🖺* for details on how to define views.
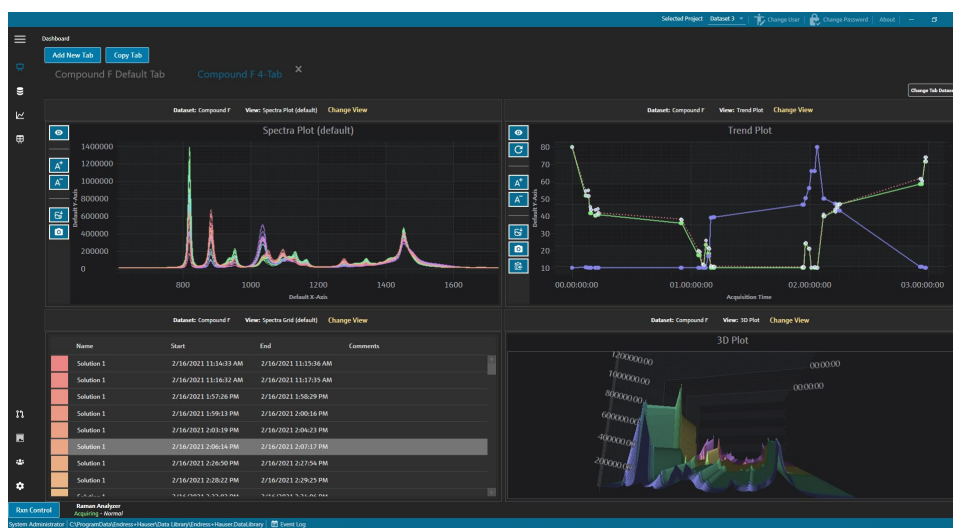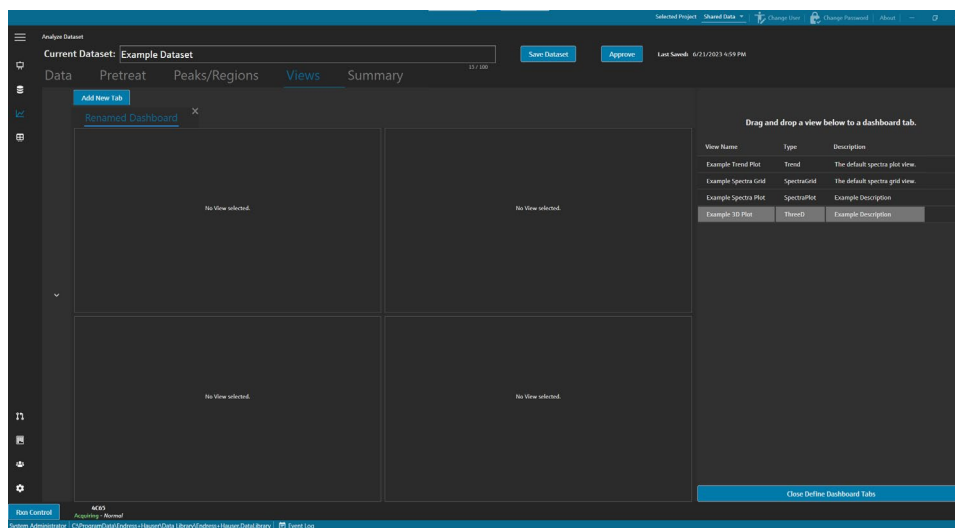


*Figure 8. 4-view dashboard tab*

From the dashboard, you can:

- **Add New Tab.** Adds a new dashboard. When adding a new dashboard tab, you are prompted to select the number of views (1 to 4). A dashboard tab can contain views from more than one dataset.
- **Copy Tab.** Creates a new copy of the current dashboard tab.
- **Change View.** Changes the view of the dataset by allowing the user to select a different plot or grid.
- **Change Tab Dataset.** Selects a dataset and remove all views from a Dashboard Tab. The selected dataset is loaded so views of plots for the selected dataset can quickly be added to the Dashboard Tab.
- **X**. Closes a dashboard tab.

**To create a new dashboard**

This procedure requires that you have added spectral sources, created a dataset from those sources, and launched an initial dashboard from the Analyze Dataset window. Refer to *Adding data to Raman data library →🖺* and *Analyzing datasets →🖺* for instructions.

1. From the dashboard, click **Add New Tab**.

   The Add New Tab list displays a selection of the number of views on the new dashboard.

2. In the **Add New Tab** list, select the number of views the new dashboard displays (1 to 4).

   When a new dashboard is created, no views of plots or grids display.

*Figure 9. Empty dashboard tab*

To create a view that shows more than the default Spectra Plot and Spectra Grid views, you need to add views on the Analyze Dataset window.

3. Define views by following the instructions in *Creating dashboard views: grids, trends, spectra, and 3D plots → 🖹*. Return to the dashboard.

4. On the new dashboard tab, click **Change View**.

   The Change view dialog displays.

5. Select the dataset source, then select the view. Click **Change View**.

The new view displays on the dashboard. To rename a dashboard, double-click the dashboard tab name.

To save a dashboard, you must define and save it in the Views tab. See *Creating dashboard views: grids, trends, spectra, and 3D plots → 🖹* for more information.

# 4 Adding data to Raman data library

This chapter provides instructions on creating data streams, spectral sources, and importing SPC files to data sets. Adding data to Raman data library can be automatic or manual. Automatic data sourcing is set up through the Spectral sources window. Manual imports of SPC files are done through the Datasets window.

There are 3 ways to bring Raman spectra into Raman data library:

- Manually import folders containing SPC files
- Auto-import SPC files from a watched folder
- Auto-import from an OPC connection to Raman RunTime

## 4.1 Projects

Projects contain and organize data. To import data into Raman data library, you must first create a project container for the data. From the Projects window, you can:

- **Add New.** Add a new project.
- **Projects Event Log.** (cGxP version only) View an event log for all projects.
- **Event Log.** (cGxP version only) View the event log for a specific project.
- **Remove.** Remove the selected project. In the cGxP version of Raman data library, the Data Remover role is required to remove a project.
- **Save.** Save a selected project.
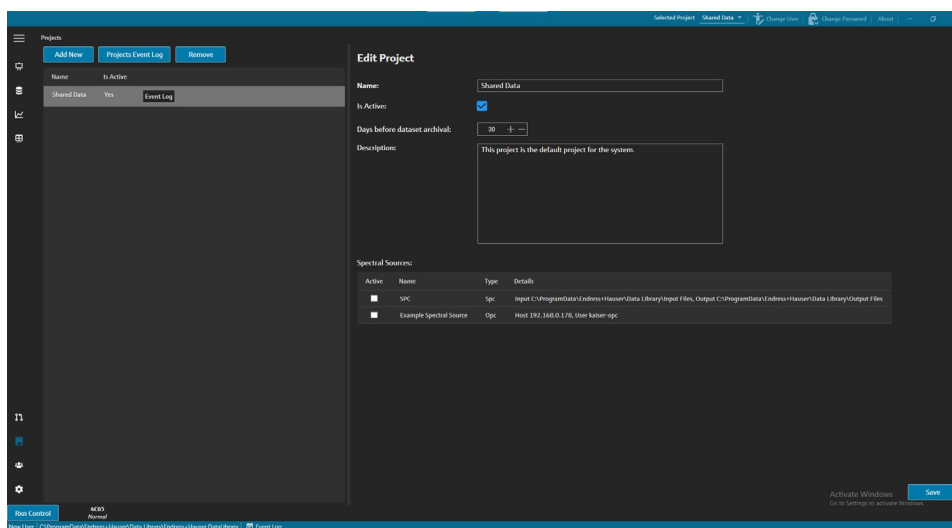


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*Figure 10. Projects window*

### 4.1.1 Adding a new project

**To add a project**

1. In the Projects window ![icon], click **Add New**.
   The Edit Project pane displays.
2. Enter the following information:
   - **Name**. The name of the project.
   - **Is Active**. Whether the project is active or not. If the Is Active checkbox is unchecked, the project does not appear in the Selected Project list on the menu bar.
   - **Days before dataset archival**. The number of days before datasets are automatically archived and are hidden on the Datasets window. Archived datasets can be viewed on the Datasets window by checking the Show Archived Datasets checkbox.
   - **Description**. The description of the project.

- **Spectral sources.** Determines which spectral sources are active for the selected project.

  Spectra, data fields, and datasets created in one project cannot be viewed in another project. However, with shared data projects, the data stored within one project can be shared with other projects. This is useful for storing reference spectra or common data fields so they can be easily included in multiple projects. To create a shared data project, select all data sources that apply to the project from the list.

3. Click **Save**.

## 4.2    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.

From the Spectral sources window, you can select:

- **Add New.** Create a new spectral source.
- **Spectral Sources Event Log**. View the event log for all spectral sources.
- **Event Log**. View the event log for a specific spectral source.
- **Remove**. Remove the selected spectral source. In the cGxP version of Raman data library, the Data Remover role is required to remove a spectral source.
- **Name.** The display name of the spectral source.
- **Type.** The type of the spectral source, either OPC or SPC.
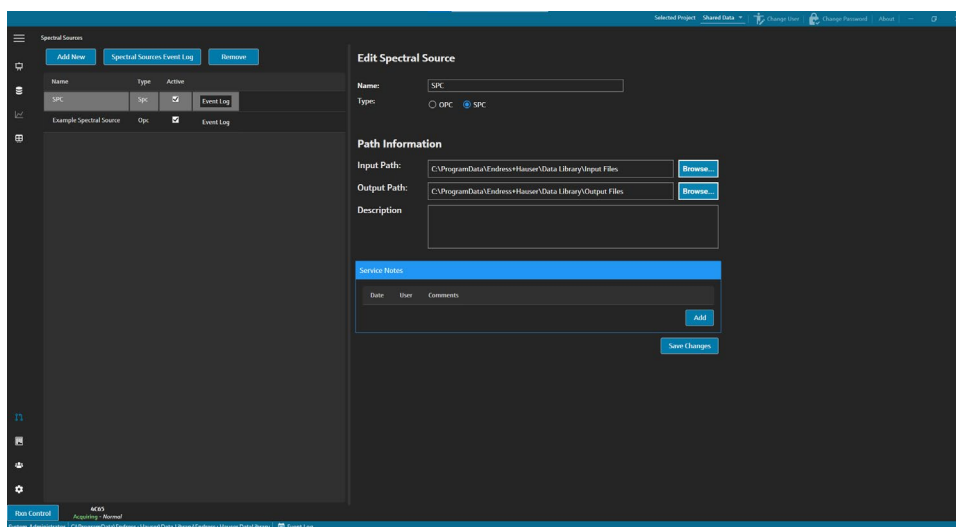


*Figure 11. Spectral sources window*

### 4.2.1    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 12. 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 of the Raman RunTime OPC server.
   - **Username**. The username used for creating the OPC connection to the Raman RunTime OPC server. The default username is **kaiser-opc**.
   - **Password**. The password used for creating the OPC connection to the Raman RunTime OPC server. The default password is **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 **Add** 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 the test connection is not successful, ensure that the Raman analyzer is powered on, available and connected to the network, and the network ports defined in *Raman Rxn2 and Raman Rxn4 network configuration* in the *Raman RunTime Operating Instructions* (BA02180C) are configured as required.
   - An unsuccessful connection may simply be due to host name resolution not configured correctly on your local IT/OT network. Please contact your local IT administrator.
   - 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.

### 4.2.2    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 also 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.
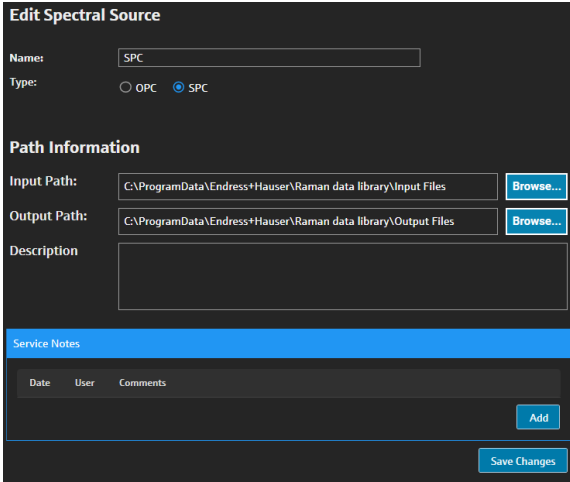
The SPC spectral source requires an input path, in which Raman data library watches for new files and imports them, and an output path, to which Raman data library moves the SPC files after they are imported.

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**. SPC files from legacy Raman software solutions need to be directed to the **Input spectra** folder.

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

   The Edit Spectral source pane displays.



*Figure 13. 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 DataLibraryBatchExport 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.

## 4.3    Datasets

The Datasets window is used to create, view, import, export, and remove datasets. Dataset summary information can be viewed for existing datasets.

In Raman data library, a dataset contains a minimum of one spectrum. Datasets can be combined for analysis or modeling within the software, or for export to external programs. To analyze spectra using a dataset, select at least 1 spectrum.

From the Datasets window, you can select:

- **Create New Dataset**. Shows the **Create Dataset** pane. In the cGxP version of Raman data library, you must have the Data Operator role to create new datasets.
- **Analyze**. Opens the selected dataset and displays the dataset on the Analyze window.
- **Import Data Library**. Imports an existing dataset file (.dlexport).
- **Export**. Displays the Export pane.
- **Remove**. Removes the selected dataset. To remove a dataset, you must be logged in under a Data Remover role.
- **Show Inactive Datasets**. Displays datasets that have been marked Inactive.
- **Show Archived Datasets**. Displays datasets that have been marked Archived. Datasets are automatically marked Archived after a configurable number of days. "Days before dataset archival" can be changed on the Projects window.
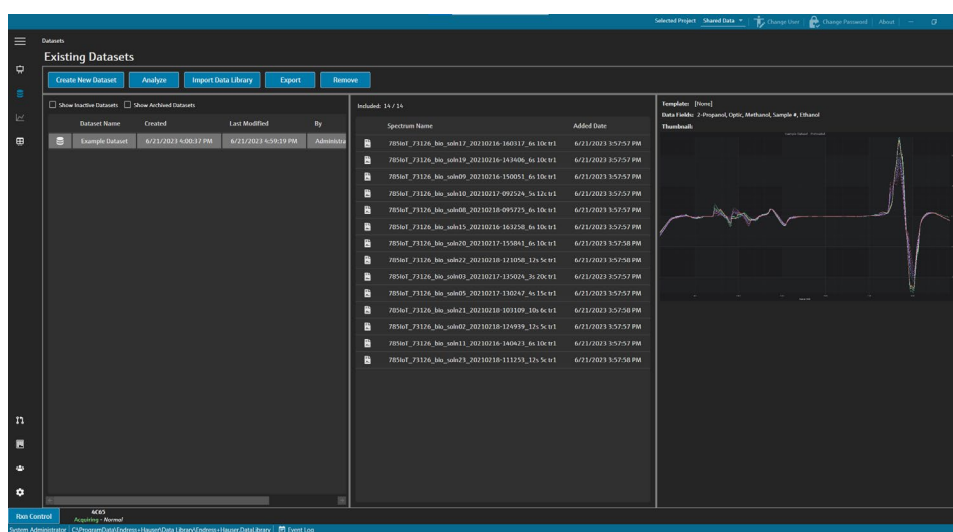


*Figure 14. Existing datasets*

## 4.3.1    Creating a dataset

You can select data from various sources to select spectra to include in a dataset. Data can be sourced from:

- **Imported Spectra**. This selection displays all available folders and spectra that have been imported into Raman data library.
- **Reference Spectra**. This selection displays all spectra that are marked as a reference spectrum.
- **Search**. This selection allows users to search for spectra that meet defined criteria. Search criteria can be added or removed individually. Spectra can be sought by a field of name, start date, end date, or any defined data values for data fields defined as searchable.
- **Existing Datasets**. This selection allows users to search for spectra that exist in another dataset. A summary view of the selected dataset is shown. When **Include ➤** is clicked, all spectra from the selected dataset is included.
- **Folders**. This selection lists spectra collected through an OPC connection to Raman RunTime, which are stored in folders located on the Raman data library computer.

Once available spectra have been selected, use **Include ➤** to include the selected spectra in the new dataset. To remove spectra from the a new dataset, select included spectra and click **◄ Remove**.
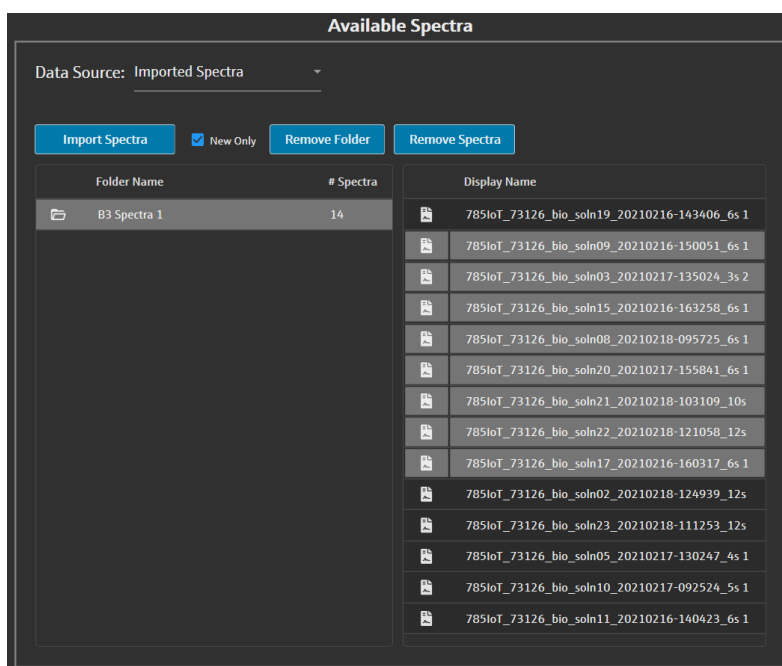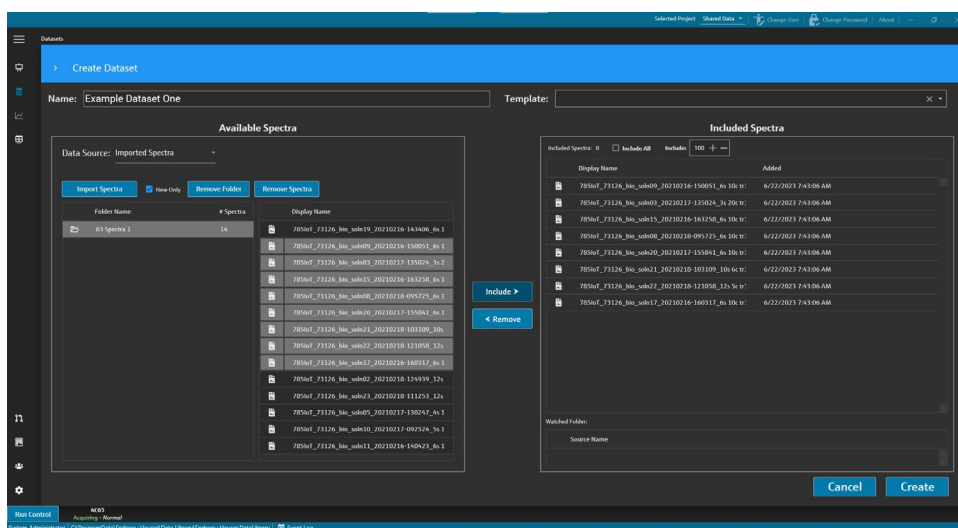
*Figure 15. Data source, imported spectra pane*

**To create a dataset**

1. On the main menu, click **Datasets** .

2. Click **Create New Dataset**.

    The Create Dataset window displays.



*Figure 16. Create Dataset window*

3. Enter the following information in the Create Dataset window:

   - **Name**. The name of the new dataset. Dataset names must be unique and have a length of 1 to 100 characters.

   - **Template**. The template to be used when creating the dataset. Templates can be used to automatically apply preselected data fields, pretreatments, peaks, regions, views, and dashboard tabs to a new dataset.

4. From the Data Source list, select:

   - **Import Spectra** to select a folder containing spectra files (.spc).

   - **Reference Spectra** to select spectra that are marked as a reference spectrum.

- **Search** to search for spectra that meet defined criteria. Spectra can be sought by a field of name, start date, end date, or other data values.
- **Existing Datasets** to search for spectra that exist in another dataset. When **Include ➤** is clicked, all spectra from the selected dataset is included.
- **Folders** to select spectra collected through an OPC connection to Raman RunTime, which are stored in folders located on the Raman data library computer. Spectra file names are not shown in the folder browser.

5. From the **Available Spectra** window, select spectra to **include**, or click **Include All** in the Included Spectra window to import all spectra in the folder.

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

6. From the **Included Spectra** window, select spectra to **remove**.
   - Select **Include All** to include all spectra from the selection in Step 5, or include only a subset of the selection in which the software selects every second or third spectra.
   - Click **Remove Folder** to remove the selected folder and all spectra within that folder. In the cGxP version of Raman data library, the Data Remover role is required to remove a folder.
   - Click **Remove Spectra** to remove the selected spectra from the dataset. In the cGxP version of Raman data library, the Data Remover role is required to remove spectra.

7. Click **Create**.

   The Raman data library workflow creates the new dataset and moves along the workflow to the Analyze window.

8. Click **Save Dataset**.

### 4.3.2    Saving a dataset

Datasets are not automatically saved in Raman data library, except when collection for a dataset is initiated from within Raman data library. It is important to get in the habit of regularly saving datasets.

Datasets can be saved through the Analyze Dataset window. If Raman data library is closed before the dataset is saved, all changes are lost.

**To save a dataset**

1. From the main menu, click **Analyze Dataset** ![icon].
2. Click **Save Dataset**.

The first time a dataset is saved it can take a few minutes. Subsequent saves are faster. After a dataset is saved, the **Last Saved** field is updated to show the last saved date and time.

### 4.3.3    Approving a dataset

Approved datasets are *read-only* and cannot be modified. The Analyze Dataset window allows you to approve or revoke approval from a dataset.

**To approve or revoke approval from a dataset**

- From the Analyze Dataset window, click **Approve** to mark the dataset as Approved.
- Click **Unapprove** to revoke the dataset approval.

## 4.4    Data fields

Data fields are qualitative and quantitative information tagged to a spectrum. For quantitative analysis, the user can specify precision, units, primary method details, and other information related to the spectrum.

Raman data library gathers preset data field information from the SPC log or OPC data sources. Units and data values displayed in the data fields list may vary depending on how the spectra are retrieved. Importing data through OPC from Raman RunTime v6.4+ auto-populates most default data fields. Aliases can be added to data fields to reduce user error during imports.

From the Data Fields window, you can add, update, and delete data fields. In the cGxP version of Raman data library, you must be logged in under a Data Fields Manager role to make changes to data fields.

From the Data Fields window, you can select:

- **Add**. Creates a new data field.
- **Remove**. Removes the selected data field. In the cGxP version of Raman data library, the Data Remover role is required to remove a data field.
- **Data Fields Event Log**. (cGxP version only) Displays the event log for all data fields.
- **Event Log**. (cGxP version only) Displays the event log for a specific data field.
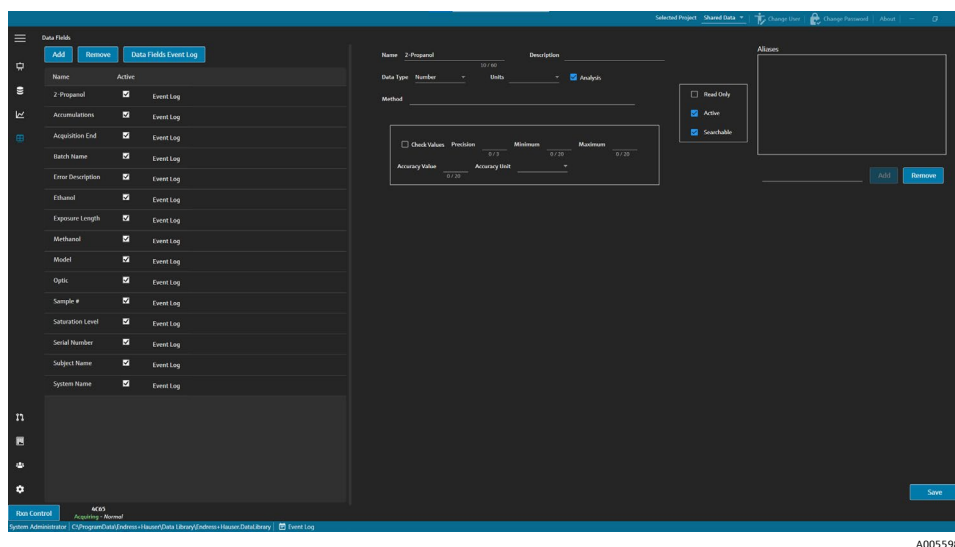- **Save**. Saves the selected data field.



A0055985

*Figure 17. Data Fields window*

**Data field properties**

| Property | Meaning |
| --- | --- |
| Name | The name of the data field. |
| Description | The description of the data field. |
| Aliases | Aliases for common variations in spelling and labeling can be added to reduce user error. For example, *Concentration*, *concentration*, and *Conc.* can be set to equal the same data field name. Adding an alias prevents common collection errors from data import and automates tagging throughout the workflow. Aliases are used on data import for matching with a column header in Excel. An alias can be added or removed here. |
| Data Type | The type of data value that can be entered for the data field:<br>▪ Boolean<br>▪ Number<br>▪ Date<br>▪ Text |
| Units | The units used for the data type. |
| Analysis | Data fields that are marked 'Analysis' can be used in analysis operations. |
| Method | A descriptive field for indicating the method of acquisition. |
| Read Only | Data fields that are marked 'Read Only' cannot have their data values altered. |

| Property | Meaning |
|---|---|
| Active | Data fields that are marked 'Active' appear on the Analysis window. |
| Searchable | Data fields that are marked 'Searchable' can be searched. |
| Check Values | Data fields that are marked 'Check Values' automatically exclude data values if they do not meet set requirements indicated in the fields Precision, Minimum, Maximum, and Accuracy Value. |
| Precision | This value designates the required number of digits past the decimal point. |
| Minimum | The lower limit for values. |
| Maximum | The upper limit for values. |
| Accuracy Value | Descriptive field indicating the accuracy value. |
| Accuracy Unit | Descriptive field indicating the accuracy unit. |

**To add a data field**

1. On the data fields window, click **Add**.
2. Enter the properties of the data field. Refer to the Data Field properties table above.
3. Click **Save**.

# 5   Analyzing datasets

The Analyze Dataset window is used to perform operations, calculations, and analysis of datasets. The analyze dataset window is made up of 5 main tabs:

- Data
- Pretreat
- Peaks/Regions
- Views
- Summary

## 5.1   Viewing datasets

The data tab is used for analysis of spectral data. The tiles on the data tab can be configured to display specific data, resized, or hidden by dragging a tile's left border to the far right.
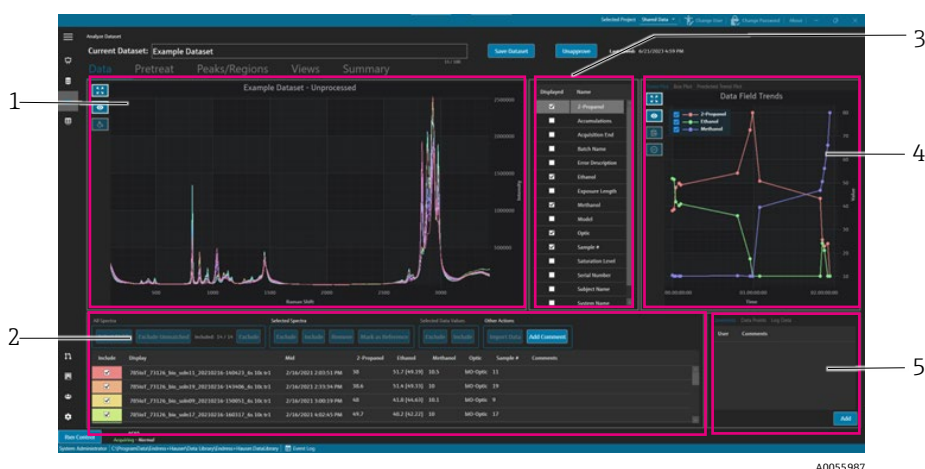


*Figure 18. Data tab*

| # | Description |
|---|---|
| 1 | **Spectra plot.** Displays unprocessed spectra included in the dataset. Colors cycle through the rainbow spectrum (pink, orange, yellow…purple, pink). |
| 2 | **Spectra grid.** Lists spectra and associated data values for displayed data fields. Provides options for including or excluding spectra and data values, and importing reference data. |
| 3 | **Data fields list.** Toggles which data fields are displayed. When on, they can be used for analysis and are listed in the spectral grid. |
| 4 | **Data fields plot.** Displays data fields as a trend plot, box plot, or predicted trend plot. |
| 5 | **Other info area.** Add comments to spectra, view log info and data points. |

### 5.1.1   Spectra plot

On the data tab, a plot of spectral data is displayed. The spectra plot shows all included spectra in their unprocessed form.

**Navigating the spectra plot**

| Navigation item | Navigation |
|---|---|
| — | Click and draw a box within the Spectra Plot to zoom into a specific area. To pan back out, double left-click the plot. |
|  | **Zoom Extents.** Zooms to the full extents of the data. This button is shown on most plots. |

| Navigation item | Navigation |
|---|---|
| <br>A0055989 | **Toggle Legend. S**hows or hides the legend. This button is shown on most plots. |
| <br>A0055990 | **Style Spectrum**. Changes the color of the selected spectrum. |

**Changing a reference spectrum name**

You can rename specific spectrum, for example, if you know the first collected spectrum is 100 % of an analyte.

1. In the spectra grid pane, select the spectra.
2. Right click, then select **Mark as Reference** or click the **Mark as Reference** button.

   The Spectrum rename required dialog displays.
3. Enter a relevant name for the reference spectra and click OK.
4. Toggle the spectra plot legend and confirm the reference spectrum is now renamed.
5. Click **Save Dataset**.

To revert a spectrum's name to its original, click **Select Fields**, then select **Name**, then **Close**. The original spectrum name appears in the list. Display names can be edited, but the original name from the collection software cannot.

**Changing a spectrum display color**

You can modify the color of a specific spectrum, for example, if you wish the reference spectrum to visually contrast with other spectra.

1. In the spectra grid pane, select the spectrum.
2. Click **Style Spectrum**  then select the desired color.

   The spectrum now displays in the styled color.
3. Click **Save Dataset**.

## 5.1.2 Data field selection

To the right of the spectra plot pane, data fields are listed. Specific data fields can be displayed or removed from the display by checking or unchecking the **Displayed** column. If a data field is marked Displayed, it can be used in analysis and is included in data export. The displayed data fields are a component of a template. See *Creating templates → 🖹* for more information.

To select data fields in the Data fields list, select **Displayed** next to the field you wish to display. The selected fields now display in the spectra grid. The first selection from the data fields list may delay before it displays. Subsequent data fields are quick to display.

The data fields list can be edited. See *Data fields → 🖹* for more information.

**To select data fields in the spectra grid**

1. Click **Select Fields** in the spectra grid.

   The field selection window displays.
2. Select the desired fields. Default fields from Raman RunTime include:
   - Name
   - Display name
   - Start date time
   - End date time
   - Midpoint date time
   - Error
3. Click **Close**.

The selected fields now display in the spectra grid.

### 5.1.3    Data field trend plot

To the right of the data fields list, a data trends graph is displayed. The data field trends plot shows spectrum data values over time.



*Figure 19. Data field trends plot*

From the data field trends pane, you can:

| Navigation item | Navigation |
|---|---|
| <br>A0055988 | **Zoom Extents.** Zooms to the full extents of the data. This button is shown on most plots. |
| <br>A0055989 | **Toggle Legend**. Shows or hides the legend. This button is shown on most plots. |
| <br>A0055992 | **Copy Plot Data to Clipboard**. Copies the current trend plot data to the clipboard. |
| <br>A0055993 | **Exclude Points**. Excludes the selected data values. |

### 5.1.4    Box plot

The Box Plot tab displays a box plot for the selected data field. The maximum, upper quartile, median, lower quartile, minimum, and standard deviation of the data field is shown. The box plot can be useful when analyzing non-sequential data samples.
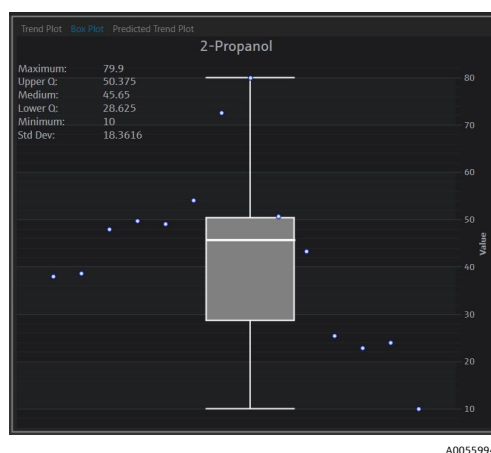


*Figure 20. Box plot*

### 5.1.5    Predicted data field trends plot

The Predicted Trend Plot tab displays predicted spectrum data values over time.



*Figure 21. Predicted data field trends plot*

### 5.1.6    Spectra grid

At the bottom of the Data tab, the spectra grid displays spectra and their associated data values for displayed fields.



*Figure 22. Spectra grid*

In the spectra grid pane, you can select spectra and fields to include. The spectra grid functionality follows.

| Spectra grid item | Display functionality |
|---|---|
| All spectra | ▪ **Select Fields**. Select which fields to display in the grid: name, display name, start date time, end date time, midpoint date time, and error. For long acquisitions it can be useful to view both start point and midpoint.<br>▪ **Exclude Unmatched**. Exclude all spectra which do not have at least one data value for the selected data fields.<br>▪ **Exclude/Include**. Exclude or include all spectra. |
| Selected spectra | ▪ **Exclude.** Exclude spectra that are selected in the spectra grid.<br>▪ **Include**. Include spectra that are selected in the spectra grid.<br>▪ **Remove**. Remove spectra that are selected in the spectra grid.<br>▪ **Mark as Reference**. Mark the first spectrum that is selected in the spectra grid as a reference spectrum. The user is required to enter a new display name for the spectrum. |
| Selected data values | ▪ **Exclude**. Exclude the selected data values.<br>▪ **Include**. Include the selected data values. |
| Other Actions | ▪ **Import Data**. Select an Excel file for data import. Opens the Import Data window.<br>▪ **Add Comment**. Add a dataset comment. The user is prompted to select a Start Date and an End Date. The comment is added for all spectra in that range. The dataset comments are specific to only the dataset in which they are added. The dataset comments are not shown in other datasets. |

**To exclude data from the spectra grid or plot**

You can exclude spectra from the grid and plot if, for example, the laser is blocked for a portion of the experiment or otherwise produces unusable data.

1. On the Spectral plot, zoom in to view only the junk data.

2. Mouse over one spectrum line in the plot and click to select it.

   The spectrum is now also highlighted in the Spectra grid.

3. Use the shift key to highlight all spectra above the selected one.

4. Click **Exclude** with the Selected Spectra box.

5. Click **Save Dataset**.

You may need to exclude a few other spectra if you did not highlight them all in the first attempt. Zooming out on the Spectra Plot should show that all the junk spectra are now excluded.

**To import data**

You can import data fields and values from an existing Excel spreadsheet.

1. In the spectra grid, click **Import Data**.

   A Select a file to import window displays.

2. Navigate to the spreadsheet and click **Open**.

   After navigating to the spreadsheet, the import data window displays.
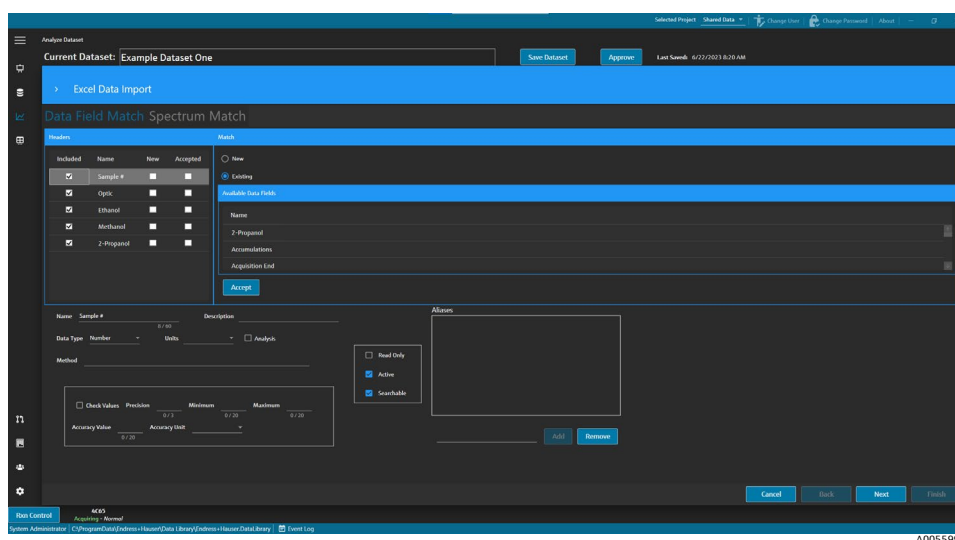


*Figure 23. Import data, data field match*

3. In the Data Field Match tab, select:
   - **Included**. Determines whether the data field with its values is imported.
   - **Match New/Existing**. Manually choose whether the selected field is treated as new or existing. If Existing, the user can choose which field it is matched with. If New, the user can edit the field in the same manner as the Data Field Editor (see above).
   - **Accepted**. Data fields can be marked Accepted for keeping track of edits.

4. Define the data field. Add a description, units, aliases, and lower and upper limits. Refer to the table describing *data field parameters →🖺* for a complete description of data field parameters.

5. Click **Next**.

6. In the Spectrum Match tab, select:
   - **Up/Down Arrows**. These arrows can be used to nudge samples up or down to line up with spectra.
   - **Threshold**. Allowable difference between the spectrum time and closest sample time (with units of Hours, Minutes, or Seconds).
   - **Apply Threshold**. Applies the threshold value to the spectra.
   - **Include Selected**. Include the selected data values.
   - **Exclude Selected**. Exclude the selected data values.
   - **Show Only Matched**. Show only spectra that have matched values.
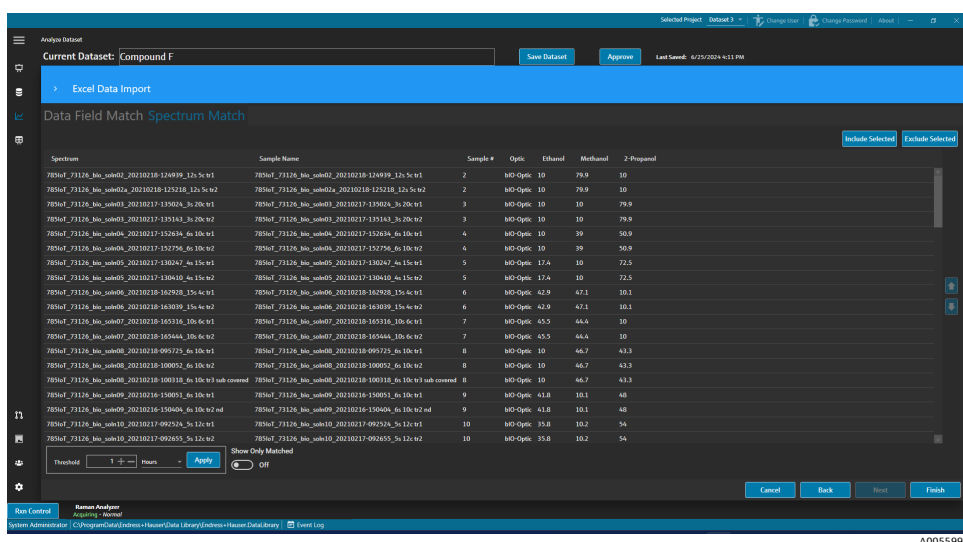
*Figure 24. Import data, spectrum match*

7. Click **Finish**. On the continue dialog, click **OK**.

8. Click **Save dataset**.

## 5.1.7   Comments

The comments tile allows you to add comments to one spectrum. These comments are not dataset-specific and are viewable in all datasets that reference the spectrum.

Comments can also be added for a dataset, or for a period of time within a dataset. This is done from the **Add Comment** button in the Spectra Grid tile. See *Modifying a spectra grid → 🖹* for more information.

**To add a comment to a spectrum**

1. In the Comments tile, click **Add**.

   The Add Comment dialog displays.

2. Enter a relevant comment and click **OK**.

   The comments tile and the spectra grid now display the comment for the selected spectrum.
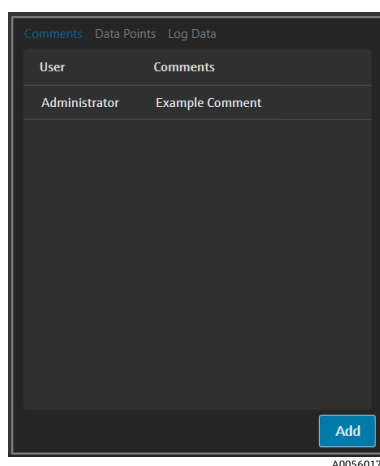


*Figure 25. Spectrum comments*

### 5.1.8    Data points

The Data Points tab displays a list of X and Y data points of the selected spectrum.

*Figure 26. Data points list*

### 5.1.9    Log data

The Log Data tab is used to view metadata (an .spc audit log) about the selected spectrum. Click **Event Log** to view the event log for the selected spectrum.

*Figure 27. Event log*

## 5.2    Using pretreatments

The Pretreat tab is used to apply pretreatments to the spectra in the dataset. Pretreatments can be removed, adjusted, and reapplied at any time and changes are reflected in the Spectra plot and in peaks and regions analysis. Pretreatments are a component of *templates* → 📖.

*Figure 28. Pretreat tab*

| # | Description |
|---|---|
| 1 | **Spectra plot**. Displays unprocessed spectra until a pretreatment is applied, then it only displays the pretreated spectra here. |
| 2 | **Spectra grid**. Lists spectra and associated data values for displayed data fields. Provides options for including or excluding spectra and data values, and importing reference data. Changing options here, such as including or excluding spectra, is reflected on the Data tab and for the next tabs in the workflow. |
| 3 | **Pretreat pane**. This is where all spectral pretreatments are applied or removed. |

Pretreatments are applied in the order they are selected to allow for sequential flexibility. The following pretreatments can be applied to a dataset:

- Click **Apply** to apply the selected pretreatment.
- Click **Remove** to remove the associated pretreatment.

### 5.2.1 Truncating

You can truncate an area of a spectra to focus on specific areas of a spectrum. Truncating crops spectra to the selected x-axis region.

**To truncate a spectra**

1. In the pretreat tab, zoom into the area of the spectra you wish to focus on by clicking on the plot and drawing a square over the area, or by clicking **Zoom** .

2. In the Pretreat pane, select **Truncate**.

3. Modify the region to crop by entering **Start X** and **End X** values. Click **Apply**.

   The Truncate pretreatment is now listed on the Pretreatment pane. Once Truncate is applied, it is no longer available in the list of pretreatments.

4. Click **Save Dataset**.

To change the truncate limits, remove any current truncate pretreatment and reapply.

### 5.2.2 Smoothing

The Smooth pretreatment applies a Savitzky-Golay based smoothing operation.

**To smooth a spectra**

1. In the Pretreat pane, select **Smooth**.

2. Select the following:
   - **Polynomial—Quadratic or Cubic.** Quadratic polynomials may be preferred when the data in a particular smoothing window approximately follows a parabolic trend. Cubic polynomials can be used to fit the local data points.
   - **Window size**. Determines how many neighboring data points are considered during the smoothing process. Adjust the window size based on the level of noise in the signal and the desired level of smoothing. Larger window sizes provide more smoothing but may also introduce more lag or distortion in the signal, while smaller window sizes capture finer details but may be sensitive to noise.

3. Click **Apply**.

   The Smooth pretreatment is now listed on the Pretreatment pane. Once Smooth is applied, it is no longer available in the list of pretreatments.

4. Click **Save Dataset**.

To change the smoothing settings, remove any current smooth pretreatment and reapply.

## 5.2.3    Applying baseline correction

Baseline Correction pretreatment removes background noise from spectra using a rolling ball, Pearson, or derivative method. You cannot apply two different baseline corrections.

The choice of method values for baseline corrections should be based on the specific characteristics of your spectral data and the nature of the baseline distortions. It can be useful to experiment with different values to find the optimal balance for accurate peak identification.

When choosing Pearson baseline correction, the values for baseline filter and fit determine the intensity or degree of baseline correction.

- **Low Fit Values (0-2)**. These values apply a gentle baseline correction. This can be beneficial if the baseline is relatively stable and you want to preserve subtle features in the data. However, it might not adequately remove all baseline distortions, potentially leading to less accurate peak identification.
- **Medium Fit Values (3-4)**. These values balance removing baseline distortions and preserving the integrity of the peaks. This is often a good starting point for many datasets, as it can improve peak identification without overly distorting the data.
- **High Fit Values (5)**. These values apply a strong baseline correction, which can be useful for data with significant baseline drift or noise. However, aggressive correction can remove or distort smaller peaks, potentially leading to missed or inaccurately identified peaks.

**To apply baseline correction**

1. In the Pretreat pane, select **Baseline Correction**.
2. Select the **Method** and related settings:
   - **Derivative**. Computes a smoothed Savitzky-Golay derivative to each spectrum.
     - **Derivative**. First or second.
     - **Polymonial**. Quadratic or cubic.
   - **Window size**. Determines how many neighboring data points are considered during the baseline correction.
   - **Pearson**. Estimates the baseline for each spectrum through iterative removal of $4^{th}$ order polynomials. This removes baseline distortions by subtracting the polynomial fit from the original spectrum.
     - **Fit type**. Polynomial, Legendre, or Hermite fit types are defined as follows:
       - **Polynomial**. Fits a polynomial function to the spectral data to model the baseline.
       - **Legendre**. Uses Legendre polynomials, which are a set of orthogonal polynomials, to fit the baseline. Legendre polynomials can minimize an error over a specific interval.
       - **Hermite**. Uses Hermite polynomials, which are orthogonal polynomials defined by a weight function involving a Gaussian distribution. Hermite polynomials can be used when data has a Gaussian-like distribution.
     - **Baseline filter (0 to 5)**. Determines the degree of baseline correction applied to the spectral data.
     - **Fit (0 to 5)**. Determines the intensity of the fitting process applied to the spectral data.
   - **Rolling ball**. Rolls a circle of fixed size under a spectrum and smoothly removes from all points of contact.
     - **Window size**. Determines how many neighboring data points are considered during the smoothing process.
3. Click **Apply**.

   The Baseline Correction pretreatment is now listed on the Pretreatment tile. Once Baseline Correction is applied, it is no longer available in the list of pretreatments.
4. Click **Save Dataset**.

To change the Baseline Correction settings, remove any current Baseline Correction pretreatment and reapply.

## 5.2.4    Normalizing

The Normalize pretreatment scales spectra to a common range. You cannot double-normalize a spectra.

**To normalize a spectra**

1. In the Pretreat pane, select **Baseline Correction**.

2. Select the **Method** and related settings:

   ▪ **SNV**. Each spectrum is normalized by removing its mean and dividing by its standard deviation.

   ▪ **Range**. Normalizes all values in a spectrum to be in the range of 0 to 1.

3. Click **Apply**.

   The Normalize pretreatment is now listed on the Pretreatment tile. Once Normalize is applied, it is no longer available in the list of pretreatments.

4. Click **Save Dataset**.

To change the Normalize settings, remove any current Normalize pretreatment and reapply.

## 5.2.5    Subtracting

The Subtract pretreatment subtracts a single reference spectrum from all spectra.

**To subtract a spectra**

1. In the Pretreat pane, select **Subtract**.

2. Select the spectrum to be subtracted in the **Spectrum** list. Click **Apply**.

   The Subtract pretreatment is now listed on the Pretreatment tile. Once Subtract is applied, it is no longer available in the list of pretreatments.

3. Click **Save Dataset**.

To change the Subtract settings, remove any current Subtract pretreatment and reapply.

## 5.2.6    Filtering intensity

The Intensity Filter pretreatment excludes spectra outside the selected y-axis minimum and maximum range. This filter is helpful if, for example, the laser is blocked or otherwise produces unusable data for a period of time.

**To filter for intensity**

1. In the Pretreat pane, select **Intensity Filter**.

2. Enter a minimum and maximum intensity range in the **Minimum Y** and **Maximum Y** fields. Click **Apply**.

   The Intensity Filter pretreatment is now listed on the Pretreatment tile. Once Intensity Filter is applied, it is no longer available in the list of pretreatments.

3. Click **Save Dataset**.

To change the Intensity Filter settings, remove any current Intensity Filter pretreatment and reapply.

## 5.3    Peaks and regions

The Peaks and Regions tab can be used to add calculations for specific x-axis ranges on a dataset. Peaks and Regions are a component of templates. See *Creating templates → 🕮* for more information.
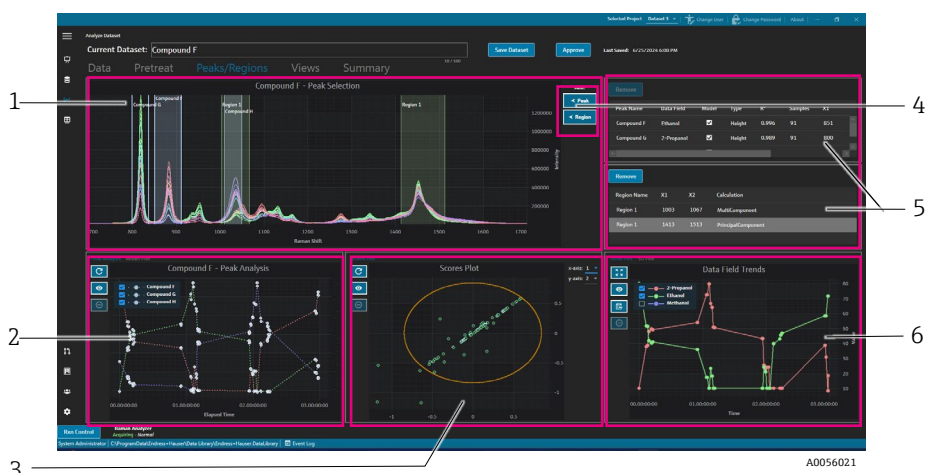
*Figure 29. Peaks and regions tab*

| # | Description |
|---|---|
| 1 | **Spectra plot**. Displays pretreated spectra. The spectra plot tile is used to select peak and region positions. In this tile, you can only zoom in or zoom out by drawing a box or by double-clicking. |
| 2 | **Peak plots**. Displays peak analysis results. In this tile, you can tab between Peak Analysis (trends) and Model plot (regression results). |
| 3 | **Region plots**. Displays results of multivariate curve resolution (MCR) or principal component analysis (PCA) when region analysis is applied. |
| 4 | **◄ Peak** and **◄ Region**. Displays a dialog for adding and defining new peaks and regions. |
| 5 | **Peak and Region lists**. Lists defined peaks and regions. You can select and edit peaks and regions in this tile. |
| 6 | **Data Field Trend plot**. The Data Field Trend plot allows you to compare peak and region results to measured data. <br> **3D plot**. Displays the Spectra plot in 3D. |

## 5.3.1 Adding peaks and regions

The peak/region selection window shows a visual representation of peaks and regions within a dataset.

**To add peaks**

1. On the Peaks/Regions tab, click **◄ Peak.**

    The Add Peak popup displays.



*Figure 30. Add peak popup*

2. Enter the **Peak Name**. This is the display name of the peak.

3. Select the **Peak Type** (height, area, or center). Center peak is useful for when peaks shift rather than grow or shrink due to a chemical or physical change.

4. Enter the range of the peak in **X1** and **X2.**

5. (Optional) Select a **Data Field** to map to the peak. The data field is used in the modeling calculation.

6. (Optional) Toggle **Model** if a model is created for the peak during export.

7. Click **Add** to create a new peak.

8. Click **Save Dataset**.

Once the peak is added, a highlighted area of the spectra plot displays. You can move, expand, or shrink the peak by moving or dragging the corners of the peak window on the spectra plot.

After creating a peak, view the peak analysis trend in the peak plot area. You can move unused windows to resize the trend plot for a larger view of trends.



*Figure 31. Spectra plot showing peak and peak analysis*

**To add regions**

1. On the Peaks/Regions tab, click ◄ **Region**.

   The Add Region popup displays.



*Figure 32. Add region popup*

2. Enter the following information:
   - The **Region Name** field is the display name of the Region.
   - The **X1** and **X2** fields are the range of the Region.
   - The **Calculation** field determines what type of calculation is done for the region (PCA or MCR).

3. Click **Add** to create a new region.

### 5.3.2 Modifying peaks and regions

**To include additional spectra in peak analysis**

1. Select the **Data** or **Pretreat** tab.

2. In the Spectra Grid, scroll to the spectrum to be included.

   You can hold down the shift key and scroll to the last spectrum to include all spectra in a range.

3. Click **Include** within the Selected Spectra box.

4. Select the **Peaks/Regions** tab and click **Refresh Plot** .

   More spectra are included in both the peak trends and spectral plot.

5. Click **Save Dataset**.

**To exclude spectra from peak analysis**

Data can be excluded directly from the trend plot. This is useful for excluding obvious outliers or when there is no change to an experiment.

1. Select the data points to exclude by clicking and dragging over the area in the Peak Analysis plot.

   The points appear bold and the exclude button is activated.

2. Click **Exclude Points** .

3. Click OK to the list of Excluded Spectra. If the points were selected on multiple peak trends, then the spectrum names may appear more than once.

4. Click **Refresh Plot** .

   Peak Analysis now only shows the data not excluded.

5. Click **Save Dataset**.
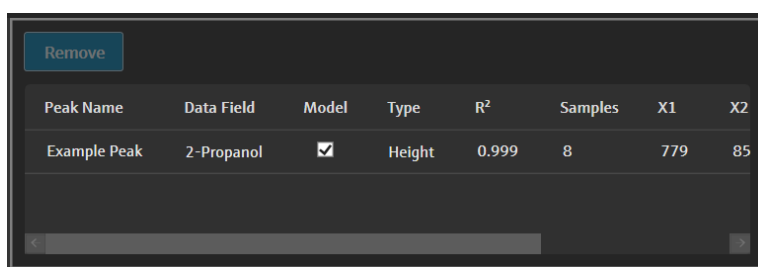
**To move and resize peaks and regions**

Peaks and regions can be moved and resized by clicking and dragging the grip handles. After a peak or region is resized, the analysis is recalculated.

**To modify or remove a peak or region**

To the right of the peaks and regions pane, peaks and regions are listed. You can view and modify the properties of a peak or region in these lists. Select a peak or region and click **Remove** to delete the selected peak or region.
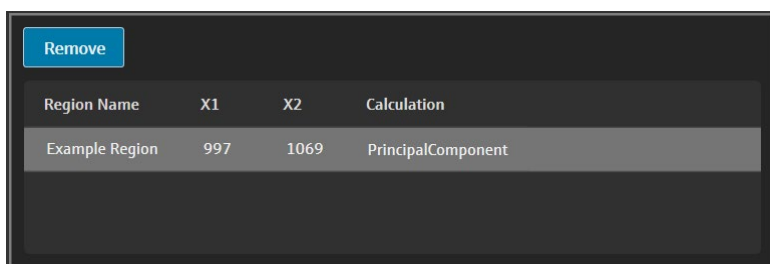
When removing a peak or region, any views using a trend generated from that peak or region should be removed or updated to a new peak or region. Failure to update or remove a trend view based on a removed peak or region results in the inability to analyze the associated dataset. Users with a view saved to their dashboard will not be able to log in if a peak or region is removed and the associated view is not updated or removed.



*Figure 33. Peaks list*



*Figure 34. Regions list*

### 5.3.3 Viewing peak analysis

The Peak Analysis tab displays a trend plot for all added peaks. Peaks are added with their own y-axis. From the Peak Analysis tab, you can:

- Click **Exclude Points** ⊖ to remove specific data points.

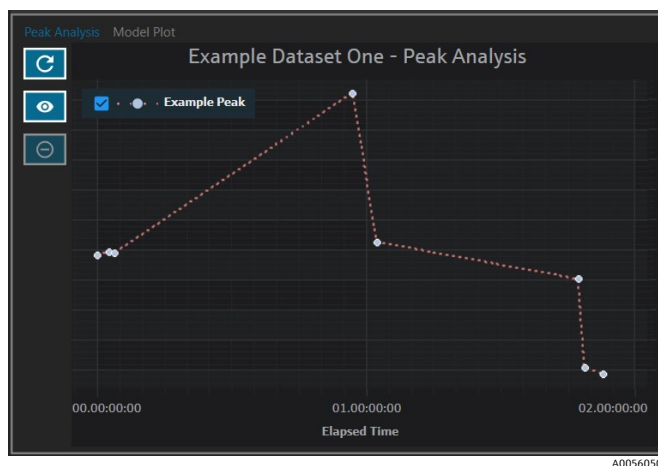- Click **Refresh Plot** ↻ to refresh the graph after modifying data points.



*Figure 35. Peak analysis*

### 5.3.4 Viewing the model plot

The Model Plot tab displays the model plot for the selected peak. From the Model Plot tab, you can:

- Click **Exclude Points** ⊖ to remove specific data points.

- Click **Refresh Plot** ↻ to refresh the graph after modifying data points. When spectra or data values are excluded from the Data tab, use the **Refresh Plot** to recalculate the model plot.
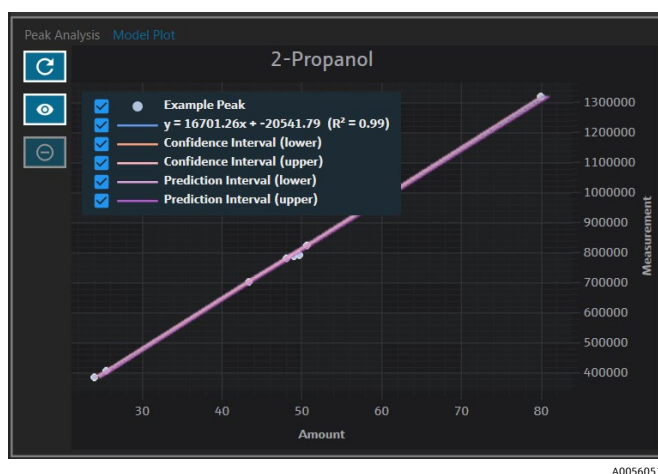


*Figure 36. Model plot tab*

## 5.4 Creating dashboard views: grids, trends, spectra, and 3D plots

The Views tab is used to define the most relevant plots and for each use case. There are many options for viewing plots, even for simple datasets. Each view can be added to a dashboard as part of a collection of views. You can create preferred dashboard tabs that display one to four plots in quadrants.

All datasets are created with two predefined views: spectra plot and spectra grid. Custom views are added, modified, and removed through the Views tab. A preview of the selected view is shown on the right side of the Views tab.

There are 4 view types:

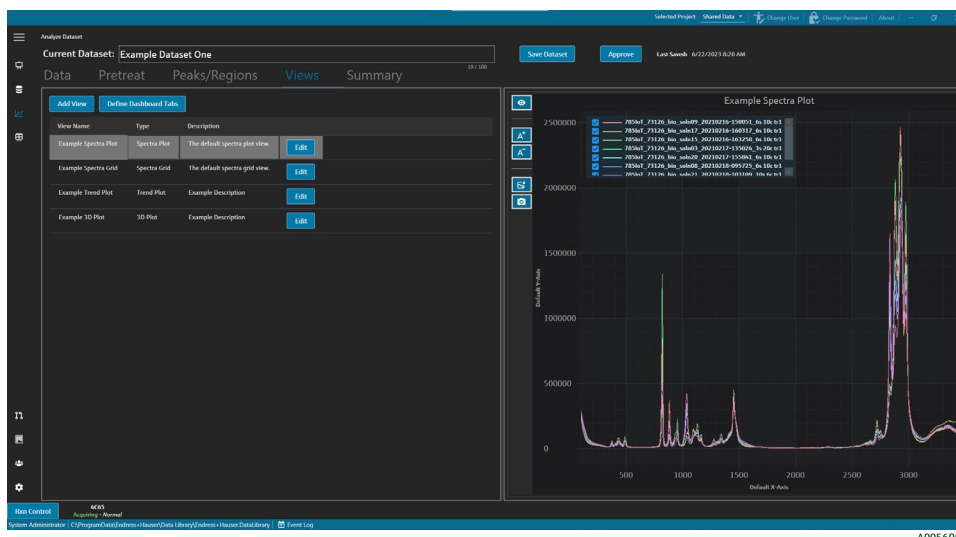- Trend plot
- Spectra plot
- Spectra grid
- 3D plot



*Figure 37. Views tab*

From the Views tab, you can also click **Define Dashboard Tabs** to open the Define Dashboard Tabs window. See *Defining a dashboard* →🗎.

To remove a view, select the view and click **Remove**. Optionally a view can be removed by selecting the view and hitting delete on the keyboard.

## 5.4.1 Creating or modifying a spectra plot view

A spectra plot view can be used to view the dataset spectra on a zoomable plot. The spectra plot is a default view that is generated for every dataset.

**To modify a spectra plot view**

1. From the Views tab, click **Add View**.

   The View Definition dialog displays.

2. Enter the following information:
   - **Name**. The display name of the view.
   - **Description**. A brief description of the view.
   - **View Type**. Select spectra plot.

3. Select the following:
   - **Use Pretreated data**. Select to show pretreated data in the view. If unchecked, the raw (not-pretreated) data shows in the view.
   - **Show latest spectrum only**. Select to show only the spectrum with the latest End Date Time. If unchecked, all spectra are shown.
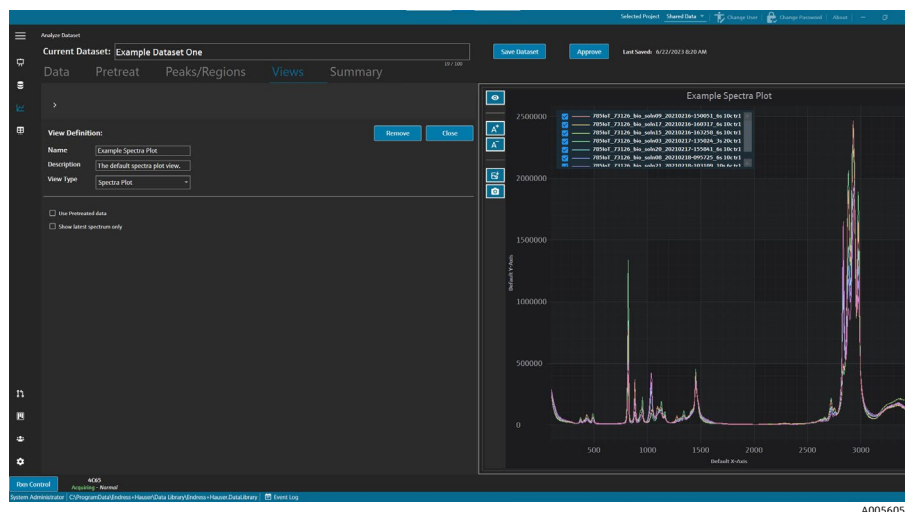
4. Click **Close**.

5. Click **Save Dataset**.

*Figure 38. Spectra plot view*

## 5.4.2   Modifying a spectra grid

The Spectra Grid view can be used to show individual spectra in a grid form. The spectra grid is a default view generated for every dataset.

**To modify a spectra grid view**

1.  From the Views tab, click **Add View**.

    The View Definition dialog displays.

2.  Select the spectra grid and click **Edit**.

3.  Enter the following information:

    ▪   **Name**. The display name of the view.

    ▪   **Description**. A brief description of the view.

    ▪   **View Type**. Select **Spectra Grid**.

4.  Click **Close**.

5.  Click **Save Dataset**.
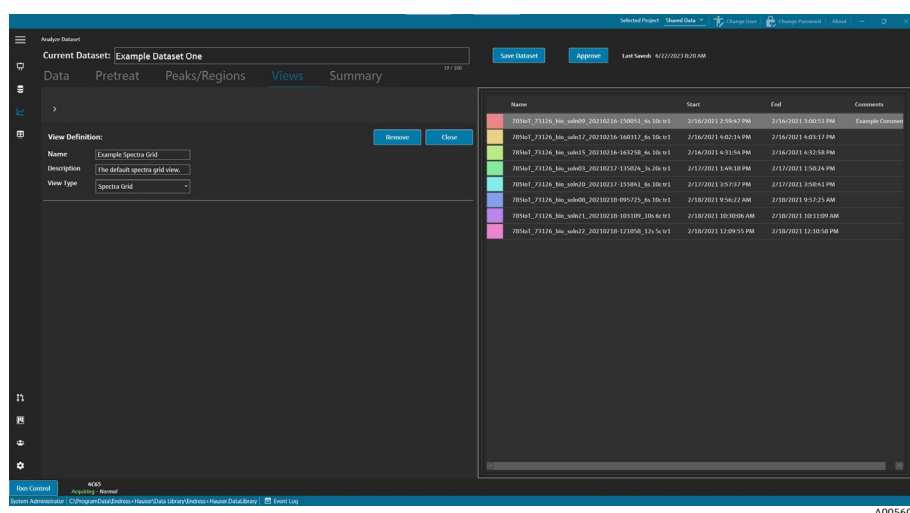


*Figure 39. Spectra grid view*

## 5.4.3   Creating or modifying a trend plot view

A trend plot view can be used to view dataset trends. In the trend plot view, the x-axis represents the relative acquisition time of the spectra. The y-axis represents the data values, predicted data values, or peak metrics.

You can choose which data fields and peaks to include in the view. When **Model** is selected for a data field that is used in a peak, predicted values are shown in the view.

**To create and modify a trend plot view**

1. From the Views tab, click **Add View**.

   The View Definition dialog displays.

2. Enter the following information:
   - **Name.** The display name of the view.
   - **Description.** A brief description of the view.
   - **View Type.** The type of view. Select **Trend Plot**.

3. From **Available data fields**, select the data fields to plot. Click **Include ➤**.

4. From **Available peaks**, select the peaks to plot. Click **Include ➤**.

5. Click **Close**.

6. Click **Save Dataset**.
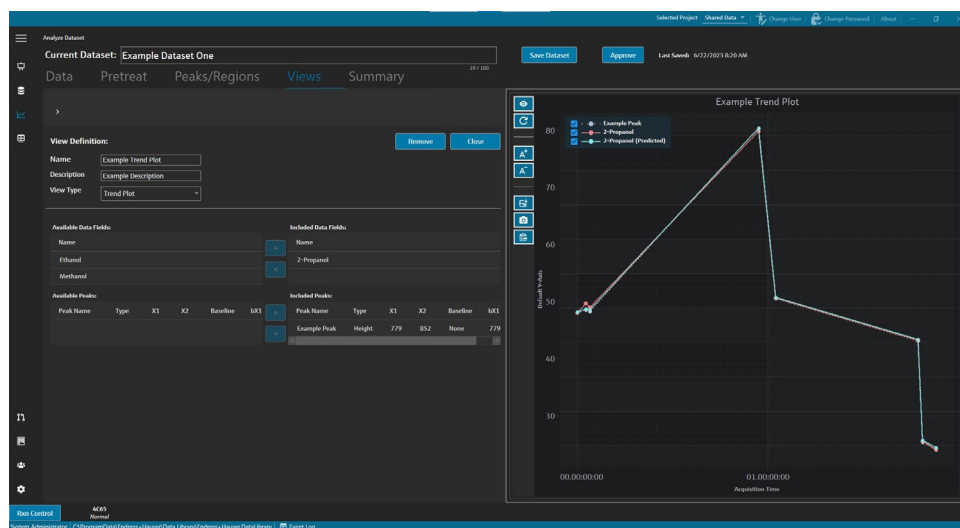


*Figure 40. Trend plot view*

## 5.4.4    Creating or modifying a 3D plot

A 3D Plot view shows the spectra in a graph with x, y, and z axes. This graph can provide additional information about the differences in spectra over time or as variables are added or removed.

**To modify a 3D plot view**

1. From the Views tab, click **Add View**.

   The View Definition dialog displays.

2. Enter the following information:
   - **Name**. The display name of the view.
   - **Description**. A brief description of the view.
   - **View Type**. Select 3D plot.

3. Adjust the plot to your desired view:
   - **Draw Contours.** Draws contour lines along a wavelength to highlight differences in spectra.
   - **Show Spectrum Colors**. Toggles spectra colors on or off, to highlight spectral changes over time.
   - **Change angle of x, y, and z axes.** The viewing angle can be adjusted by clicking on the plot and dragging to the desired position.
   - **Zoom in or out**. The mouse wheel zooms the plot in and out.

4. Click **Close**.

5. Click **Save Dataset**.
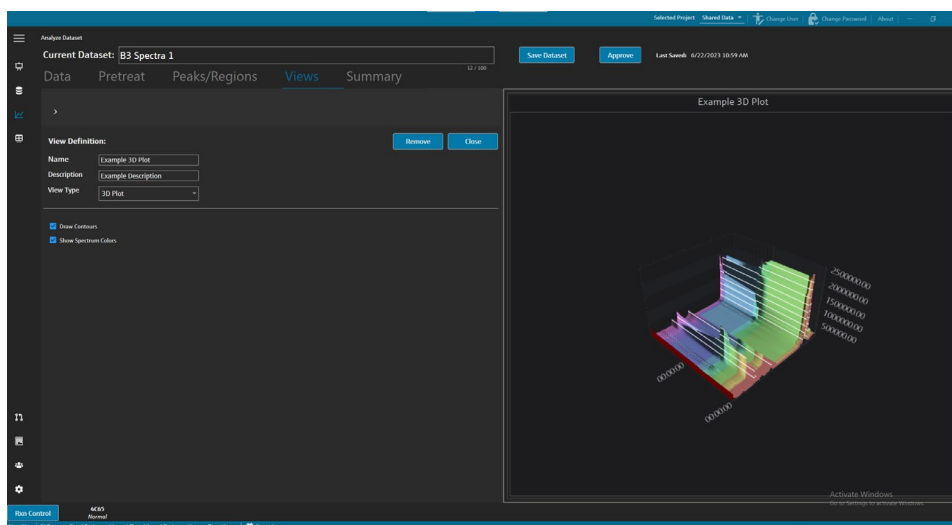


*Figure 41. 3D plot view*

### 5.4.5    Adding temporary annotations

In the Views tab, you can create temporary annotations including highlighted areas, labels, lines, and arrows. Then you can save the annotations with the view to refer to later or to share.

In the Views tab, you can:

| Navigation item | Navigation |
|---|---|
| A⁺ A0056085 | **Add Temporary Annotation.** Adds a temporary annotation to the view. |
| A0056086 | **Save Image File**. Saves the view with annotations. |
| A0056087 | **Copy Image to Clipboard**. Copies the current view with annotation to the clipboard. |
| A0055992 | **Copy Plot Data to Clipboard**. Copies the current trend plot data to the clipboard. |
| A⁻ A0055993 | **Remove Temporary Annotation.** Removes a temporary annotation from the view. |

**To create temporary annotations**

1. From the Views tab, select a view you wish to annotate.

2. Click **Add Temporary Annotation** [A⁺] .

3. Select the **Annotation type**:
    - **Line**. Places a line on the view.
    - **Line arrow**. Places an arrow line on the view.
    - **Text**. Places text on the view.
    - **Box**. Places a highlighted box on the view.
    - **Horizontal line**. Places a horizontal line on the view.
    - **Vertical line**. Places a vertical line on the view.
    - **Axis Marker**. Places an axis marker on the view.

4. Click **Add Temporary Annotation** then click the view to place the marker.

5.  Save the view by doing one of the following:

    ▪   Click **Save Image File** [icon] to save the view with annotations.

    ▪   Click **Copy Image to Clipboard** [icon].

    ▪   Click **Copy Plot Data to Clipboard** [icon].

6.  Click **Save Dataset**.

### 5.4.6    Defining a dashboard

From the Views tab, you can define and save a dashboard. To do this, you must first create views that were outlined in the previous sections. By default, the Views tab contains a Spectra Plot and Spectra Grid view for each dataset.

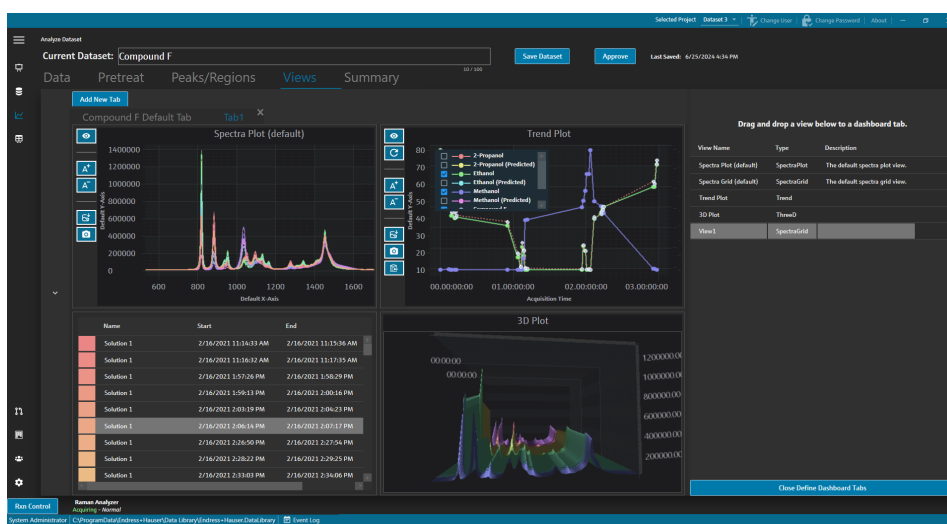**To define a dashboard**

1.  From the Views tab, click **Define Dashboard Tabs**.

    A default tab for the current dataset displays, showing the Spectra Plot and Spectra grid.

2.  Click **Add New Tab**.

    The Add New Tab popup displays.

3.  Select the number of views to display:

    ▪   1-View Tab
    ▪   2-View Tab
    ▪   3-View Tab
    ▪   4-View Tab

    A new dashboard displays.
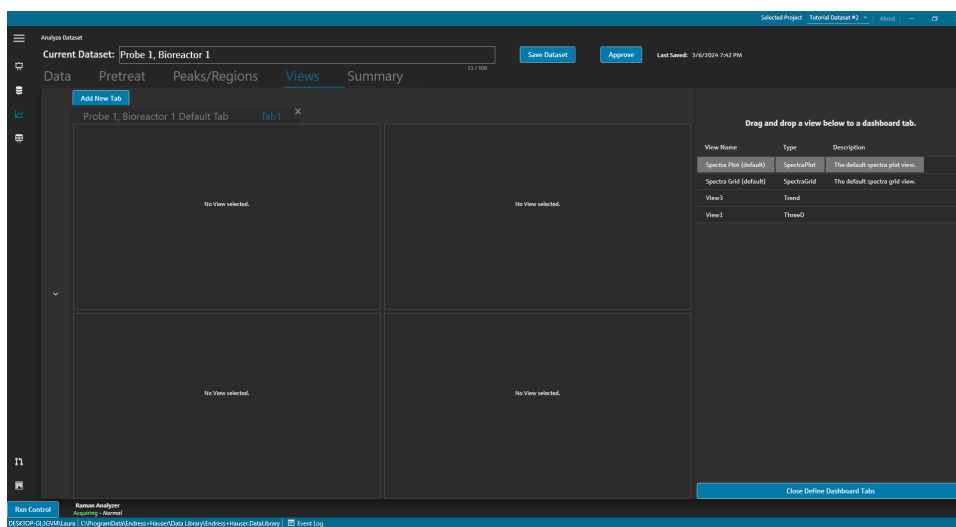


*Figure 42. Defining a new dashboard*

4.  Drag and drop the desired views from list on the right to the desired area of the dashboard.

*Figure 43. Selected views on a new dashboard*

5. Double-click the tab name and rename the dashboard as desired.

6. Click **Save Dataset**.

7. Click **Close Define Dashboard Tabs**.

## 5.5 Summary

Datasets are summarized and analysis is applied in the Summary tab. The Summary tab is also where templates are saved, Raman data library model files are exported, and where datasets can be exported for external modeling.

In the Summary tab, you can:

- **View summary information** about the dataset. Summary information indicates the status of the dataset, its approval state, the total spectra included, and applicable data fields. Pretreatments, peaks, regions, and a snapshot of the plot are also displayed.

- **Export the dataset.** Click **Export** to export the current dataset. Refer to *Exporting data, datasets, and models →🗎* for more information.

- **Launch dashboard tabs.** Click **Launch Dashboard** to add a copy of the dataset's dashboard to the dashboard window. The dashboard is defined in the Views tab. Refer to *Creating dashboard views: grids, trends, spectra, and 3D plots →🗎* for more information.

- **Create templates** from the dataset. Refer to *Creating templates →🗎* for more information.

- **View events** related to the dataset. Click **Dataset Event Log** to view the event log for the current dataset.
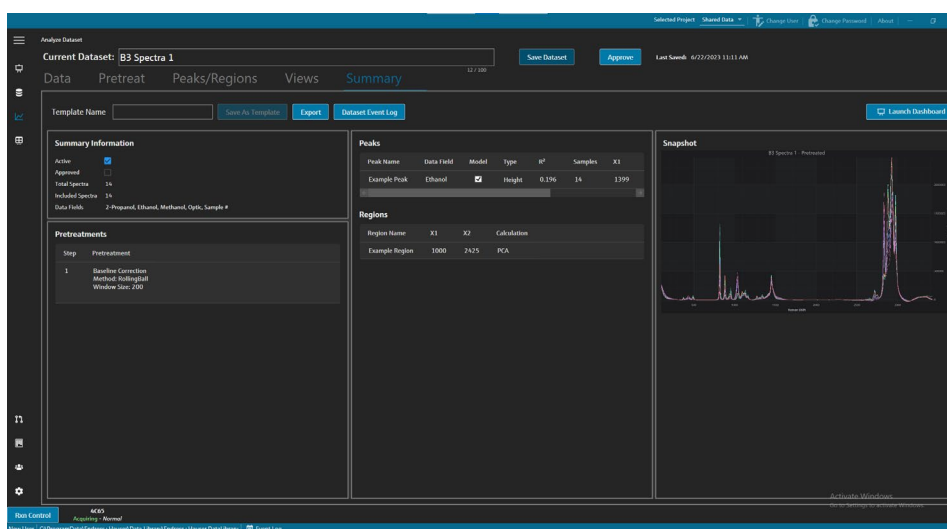


*Figure 44. Summary tab*

### 5.5.1    Creating templates

When components of a dataset can be reused in other datasets, templates simplify dataset creation. Templates store all pretreatments, analysis, and view settings and can be applied to new datasets. A template contains the following:

- Displayed data fields
- Pretreatments
- Peaks
- Regions
- Views
- Dashboard tabs

A template does not contain spectra data.

Saved templates can be selected on the Create Dataset window when creating a new dataset, or on the Rxn Control window. If a template is selected during dataset creation, all components of the template are added to the new dataset.

**To create a template from the current dataset**

1. Select the **Summary** tab.
2. Enter a name in the **Template Name** field.
3. Click **Save As Template.**
4. Click **OK**.

### 5.5.2    Applying templates

When creating a new dataset, you can apply a template.

**To apply a template**

1. From the Datasets  window, click **Create New Dataset**.
2. Name the dataset, import the corresponding spectra, and click **Include >**.
3. In the **Template** field, select the template from the list.
4. Click **Create**. If you get a prompt to save an unsaved dataset, click OK.

When complete, Raman data library moves along the workflow to the Analyze Dataset window.

### 5.5.3    Exporting data, datasets, and models

The Export pane is used to export Raman data library datasets to external and internal software systems. A Raman data library export file (.dlexport) can be used to move datasets from one instance of Raman data library to another. For exporting to external software systems, the dataset must be approved.

**To export data, a dataset, or a model**

1. From the **Datasets** window , click **Export**.
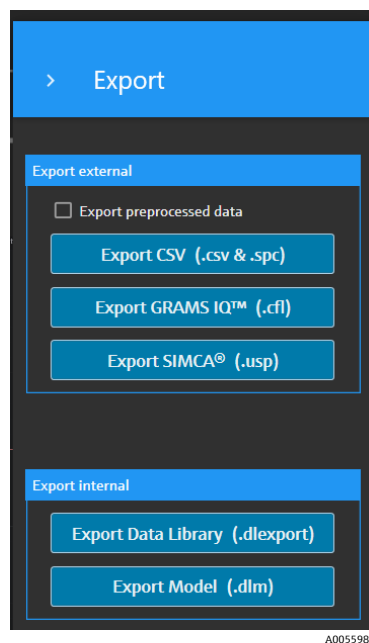
    The Export menu displays.

*Figure 45. Export menu*

2. Select the following options:

   - **Export preprocessed data.** When checked, the data is exported without pretreatments applied.

   - **Export CSV.** Exports the dataset as a comma separated values file (.csv) containing spectra names and data values for all included data fields. Also exports a zipped folder containing the included spectra in SPC (.spc) form.

   - **Export GRAMS IQ™.** Exports the dataset as GRAMS IQ™ (.cfl) file. Also exports the included spectra in SPC (.spc) form. A valid GRAMS IQ™ installation on the same computer as Raman data library is required to be able to export as a GRAMS IQ™ (.cfl) file.

   - **Export SIMCA®.** Exports the dataset as a SIMCA® (.usp) file. A valid SIMCA® installation on the same computer as Raman data library is required to be able to export as a SIMCA® (.usp) file.

   - **Export Data Library.** Exports the dataset as a Raman data library (.dlexport) file. This file type can be imported on the Datasets window.

   - **Export Model.** Exports a model file (.dlm) that is created using the pretreatments and peaks of the dataset. This file can be exported to Raman RunTime using the Raman data library Rxn Control window. The model file can be used to generate component process values in RunTime.

3. Navigate to the folder location and name the data file.

4. Select **Mark Inactive** or **Keep Active** for the current dataset.

# 6    Raman Rxn analyzer control

Rxn Control is used to manage Raman RunTime Rxn analyzers for Raman spectra collection and modeling and is designed to mimic the Raman RunTime user interface. To access the Raman Analyzer window, an OPC spectral source connection must be created. Refer to *Adding an OPC spectral source* →🗎 for instructions.
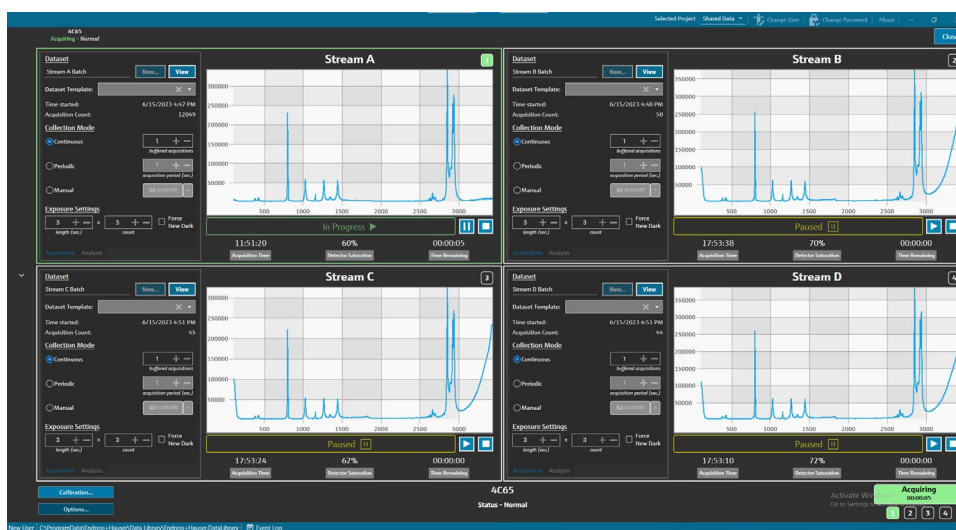
> **NOTICE**
>
> **For information about the safe operation of Raman Rxn analyzers and the Raman RunTime software, view the *Raman RunTime Operating Instructions* (BA02180C).**

▶  Depending on the version of Raman RunTime you are using, read the corresponding *Raman RunTime Operating Instructions* before using the Raman data library Rxn Control.



*Figure 46. Rxn Control button*



*Figure 47. Raman Analyzer window*

The **Rxn Control** button is only present when a Raman Rxn analyzer is connected to Raman data library. To connect an analyzer, refer to the instructions in *Adding an OPC spectral source* →🗎.

## 6.1    Analyzer options

The **Analyzer Options** menu is accessed by clicking **Options** at the bottom of the **Raman Analyzer** window.
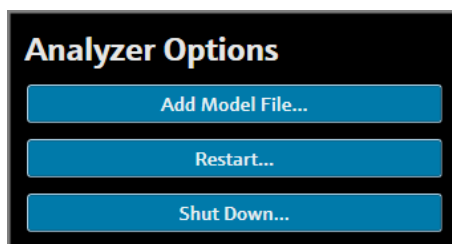


*Figure 48. Rxn analyzer options*

### 6.1.1    Adding a model file

**To add a model file:**

1.  From the **Rxn Control** window, click **Options**.

    The Analyzer Options dialog appears.

2.  Click **Add Model File** to select a model file to send to Raman RunTime.

    Added model files can be used for analysis. They are enabled or disabled by clicking the **Analysis** tab on a probe window. Valid file types include: .usp, .rusp, .dlm, .pxm, .pxs, .cal, .mat, and .unsb files. For details on Raman RunTime's supported model types, refer to the *Raman RunTime Operating Instructions* (BA02180).

For instructions on restarting or shutting down the analyzer, see *Restarting or turning off the analyzer* →🖺.

## 6.2      Channel control

Raman Rxn analyzers can have up to 4 probes, or measurement channels, in the Rxn Control window. Each channel has a control pane on the Raman Analyzer window. Use the channel pane to select and view datasets, set collection modes, set exposure settings, and more.

Each channel pane contains settings that reflect Raman RunTime operations. For complete descriptions of the functionality found in a channel pane, refer to the *Raman RunTime Operating Instructions* (BA02180).
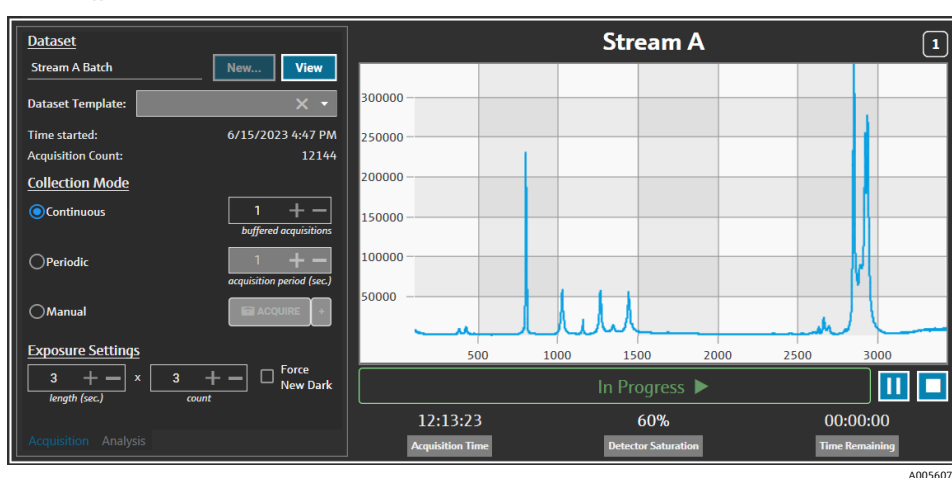
### 6.2.1      Channel acquisition



*Figure 49. Channel control pane*

From the channel **Acquisition** tab, select:

- **New.** Creates a new named dataset.
- **View.** Launches the current dataset on the Dashboard window.
- **Dataset template.** Select a template to apply to the new dataset. A template must be selected before a batch is started.
- **Time Started.** The time (in seconds) that has passed since the current dataset was started.
- **Acquisition Count.** The number of acquisitions for the current dataset.
- **Collection Modes.** The probe collection mode can be changed by selecting one of three options:
  - **Continuous.** Continuous collection mode cycles through each active probe as quickly as possible. This setting is recommended for method development when collecting frequent reference samples, and for monitoring and control when models are active. Continuous mode includes a buffered acquisition option.
  - **Periodic.** Periodic collection mode acquires spectra at specified intervals and is typically used during method development to allow spectra to sync with samples being drawn from reactors or other timed process events. Buffered acquisitions are not an option in periodic mode.
  - **Manual.** Use the Manual collection mode to acquire spectra that are triggered manually by the 📷**Acquire** button. Sample names can be specified for each spectrum by clicking **+**.
- **Exposure Settings.** The exposure settings of length (seconds) and count can be changed by clicking **+** and **−** or by manually typing a value with the keyboard. Select **Force New Dark** to force a new dark exposure after every acquisition.

    Collecting a new dark exposure can mitigate non-sample contributions in the measurement due to dark current. For more information on Force New Dark, refer to the *Raman RunTime Operating Instructions* (BA02180).

*Figure 50. Exposure settings*

## 6.2.2    Applying models on the channel Analysis tab

The channel **Analysis** tab enables you to select and apply models within Raman RunTime to receive model predictions during dataset acquisition.
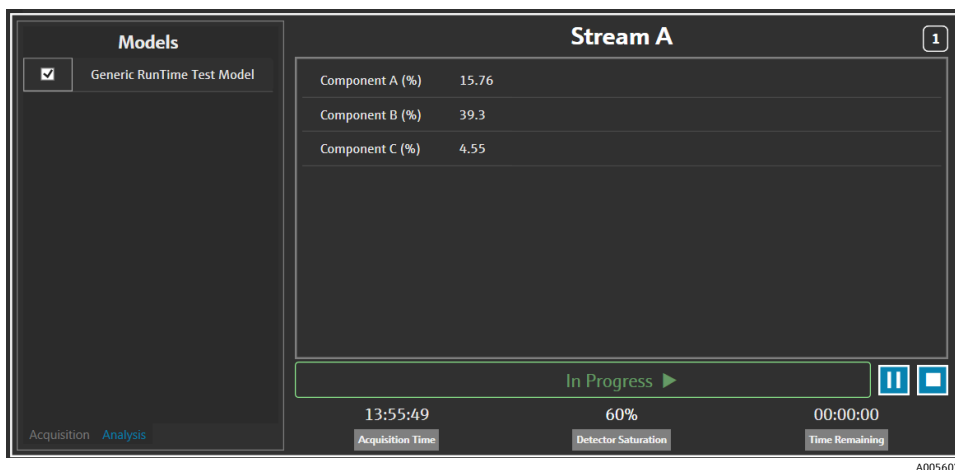


*Figure 51. Channel control analysis tab*

To choose a model, check the model file name. The following information displays:

- Predicted values display on the Analysis tab.
- Raman RunTime model predicted results display in square brackets on the Analyze window, for example [8.14].

## 6.2.3    Acquiring spectra

To start dataset acquisition, click **Play** ▶. After dataset acquisition has started, the play button changes to a pause button.

Click **Stop** ▣ to stop dataset acquisition.

## 6.2.4    Channel status bar

The channel status bar is shown under the spectrum plot. A channel can have a status of Not Started, In Process, Paused, or Completed.
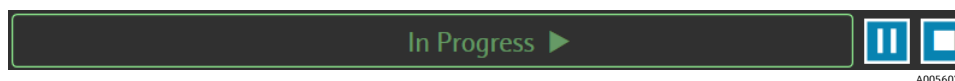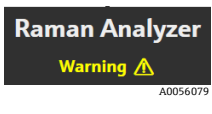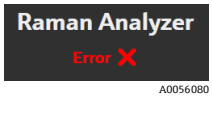


*Figure 52*. Channel Status Bar

## 6.2.5    Analyzer status and action indicators

The analyzer status indicator is shown at the bottom-center of the Rxn Control window. There are three analyzer statuses: Normal, Warning, and Error.

| Status | Description |
|---|---|
|  | The status is normal. |

| Status | Description |
|---|---|
| Raman Analyzer Warning ⚠ A0056079 | If a system warning is encountered, the display changes to a Warning in yellow. Warnings should be acknowledged but immediate action may not be necessary. Click the status to view details of the warning. |
| Raman Analyzer Error ✗ A0056080 | If a system error is encountered, the display changes to an Error in red. Errors require immediate action. Click the status to view details of the warning. |

Refer to the *Raman RunTime Operating Instructions* (BA02180) for a full listing of system warning and errors.

## 6.2.6 Analyzer action indicator

The analyzer action indicator is shown in the bottom-right of the Rxn Control window. The indicator shows the current action being performed. If the action is channel-specific, the affected channel number flashes. In case of an emergency, the red stop button in the indicator cancels the currently occurring Calibration or Verification process.
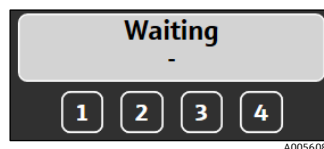


*Figure 53. Acquiring spectra*



*Figure 54. Paused or waiting for user input*



*Figure 55. Calibrating (probe or internal)*



*Figure 56. Verifying probe*

## 6.3 Raman Rxn analyzer calibration and verification

Raman Rxn analyzer control through Raman data library does not allow spectra to be collected without passing internal and probe calibrations. All calibrations are required prior to spectral acquisition. Verification is optional but recommended.

For complete instructions on calibrating or verifying a Raman Rxn analyzer or probe, refer to the applicable probe calibration kit instructions and the *Raman RunTime Operating Instructions* (BA02180).

**To perform Rxn analyzer calibration and verification:**

1. From the **Raman Analyzer** window, click **Calibration**.

   The Calibration dialog opens.

2. Select Internal Calibration options:
   - **Calibration Mode.** The calibration mode for internal calibration (Auto, XAxis, or All).
   - **Laser Power**. The power of the laser in mW.
   - Click **Calibrate** to perform an internal calibration.
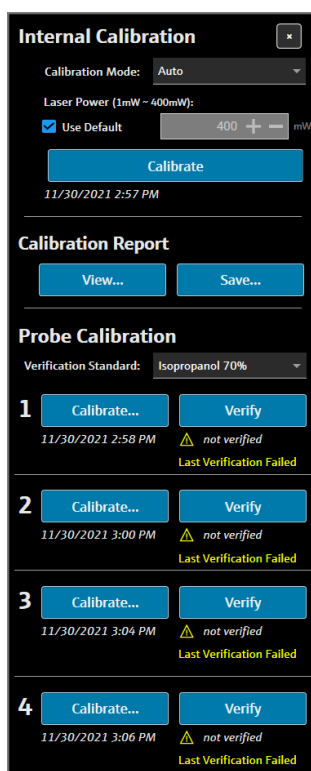


*Figure 57. Calibration dialog*

3. Select Calibration Report options:
   - Click **View** to view the calibration file (.pdf).
   - Click **Save** to save a copy of the calibration file (.pdf).

4. Select Probe Calibration and Verification options:
   - **Verification Standard.** The standard reference sample used for verifying the probe calibration results. While this step is not required to collect a Raman spectrum, it is highly recommended.
   - Click **Calibrate** under a channel to perform open the probe calibration window. Follow the calibration instructions and click **Load** to select an Intensity Reference file to use for the probe calibration. Click **Save** to save a copy of the selected Intensity Reference file.

     Use of the Raman calibration and verification kit with a Calibration Reference Standard (CRS)-based source spectral file is currently not supported through the Raman data library Rxn analyzer control interface.
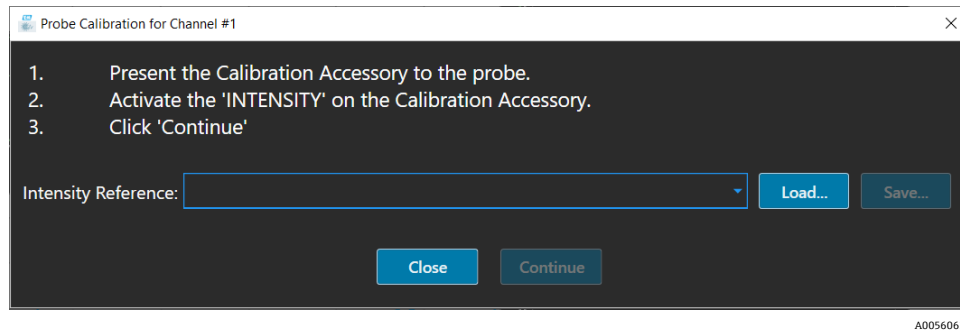
A0056061

*Figure 58. Probe Calibration window, HCA*

- Click **Continue** to start the probe calibration. After probe calibration has been completed, the calibration date/time updates.
- Click **Verify** to verify the probe calibration results.

5. Repeat the above steps for each analyzer and probe.

6. When calibration and verification is complete, close the calibration dialog.

# 7 FDA 21 CFR part 11 compliance

The cGxP version of Raman data library features added functionality for FDA 21 CFR part 11 compliance. These features support a centralized implementation of 21 CFR part 11 requirements, enabling a regulated process setting. The cGxP version of Raman data library includes support for:

- User management
- Electronic records and electronic signatures
- Managing system settings
- Audit trail (change control function)
- Event logs that include user action traceability and spectral data traceability

To support 21 CFR Part 11 implementations of Raman data library cGxP, Endress+Hauser has made available a dedicated document, Raman data library 21 CFR Part 11 Questionnaire (p/n 4005768) that is delivered with the cGxP version of Raman data library.

## 7.1 User management

In 21 CFR Part 11, user management pertains to the set of controls and procedures that ensure secure and regulated access to electronic records and electronic signatures. One of the main differences between Raman data library's core version and cGxP version is user management. In support of this Raman data library cGxP has integrated user management, credential authentication of which can be local in nature i.e. through the software itself, through local Windows workstation logins, or through a tie into an Active Directory domain.

When a local authentication mode is utilized, the ability to enforce password complexity aspects is supported as well as lockout after a set number of login failures and automatic timeout. If domain-based credential authentication is utilized, all these aspects except software timeout are governed by the domain instead.

Unique user identification and access control are natively deployed. User access privileges can be configured with set and controlled user roles. The ability to disable accounts and enforce a password change at next login is also available. User specific audit trail in the form of event logs is present.

User management within Raman data library is implemented in a way that helps ensure electronic records are secure, access is controlled, and all user actions are traceable, supporting the reliability and integrity of data in regulated industries.

For details on managing users, see *User Management (cGxP version only)* →🖺.

## 7.2 Electronic records and electronic signatures

Electronic records and electronic signatures are fundamental components of 21 CFR Part 11, which establishes the criteria under which they are considered trustworthy, reliable, and equivalent to paper records and handwritten signatures. Electronic signatures within Raman data library are linked to individual users and their credentials, making them legally binding and non-repudiable.

To aid sites with 21 CFR Part 11 implementation of Raman data library and specifically on the topic of electronic records and electronic signatures, Endress+Hauser has made available a dedicated document, Raman data library 21 CFR Part 11 ER/ES Assessment (p/n. 4005770) that is delivered with the cGxP variant of the software.

## 7.3 Managing system settings

System settings within Raman data library pertain to security aspects that play a critical role in helping achieve 21 CFR Part 11 compliance. System settings are managed in the Security window. For details on managing security settings, *refer to Security settings (cGxP version only)* →🖺.

## 7.4 Audit trail through change control function

Audit trail is a critical component of 21 CFR Part 11 compliance, ensuring that any changes to electronic records, systems, or processes are properly managed and documented.

In the cGxP version of Raman data library, as a tie-in to user management, a change control function has been implemented. This ensures that all changes are documented including the reason for the change, the date and time, and the individual responsible for making and approving the change. An audit trail of the changes is tracked and documented within the various event logs available. In addition, the change control function ensures that only people with appropriate authorization are allowed to make any updates or modifications.

Certain actions, such as removing or unapproving datasets and adding, editing, or removing data fields, removing projects or spectral sources require the user to sign off before the action can be implemented. Where appropriate the user is required to sign-off with their credentials and select a reason for the change with a space for any associated comments.
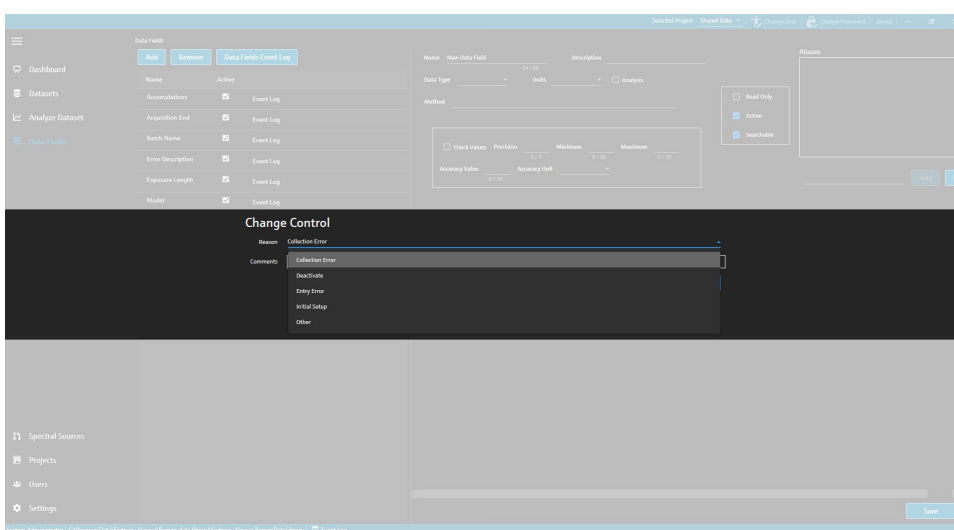
The default reasons available for change control are:

- Collection Error
- Deactivate
- Entry Error
- Initial Setup
- Other
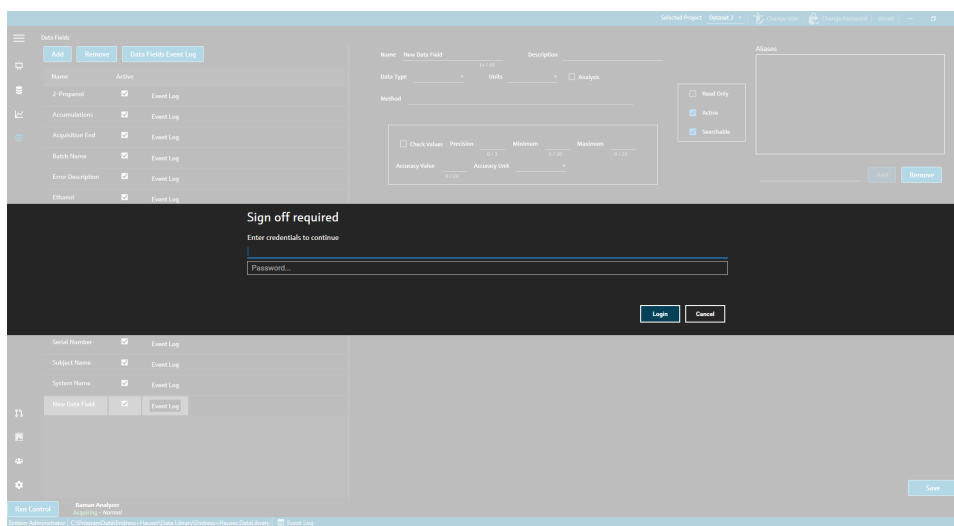


A0056145

*Figure 59. Change control–user signature required*



A0056146

*Figure 60. Change control–providing a change description and reason*

These change control measures help maintain the integrity, reliability, and compliance of electronic records and systems, and helps with approval and audit processes by a Quality team.

## 7.5 Working with event logs

To ensure traceability and logging of all events in a cGxP environment, Raman data library features event logs that include a basic audit trail. These range from global (all actions) to user or feature-specific event logs. Event logs and audit trails are essential components of 21 CFR Part 11 compliance, ensuring the integrity and traceability of electronic records.

The various kinds of event logs where a user can view events in Raman data library are:

- **Global event log.** This event log can be accessed from all screens in Raman data library and is in the bottom taskbar of the application window.
- **User event logs.** Displays events for all users, or a specific user. This is accessed from the Users screen.
- **Project and dataset event logs.** Displays events for all projects, or a specific project, and lists events related to a dataset. These logs are accessed from the Projects screen and the dataset summary screen.
- **Spectral source event logs.** Displays the event log for specific spectral sources or all spectral sources.
- **Data field event logs.** Displays the event log a specific data field, or for all data fields.

Event logs can be viewed and printed in an easily viewable, unmodifiable, and proprietary document format. Searching for text within the log is supported. Before opening another event log, the current event log must be closed. For viewing purposes only, event logs can be saved as *.pdf, *.xlsx, and *.docx.

### 7.5.1 Global event log

The global event log displays all events on an implementation of Raman data library. Due to the breadth of logged information, the global event log may take some time to load.
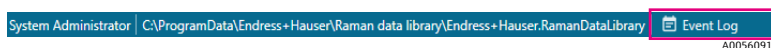


*Figure 61. Global event log button*

### 7.5.2 User event log

From the Users window, you can view event logs that list events related to a specific user, or all users. This log collects all changes to users, including adding or removing users, adding or removing roles for a user, user logins, and failed login attempts. From the Users window, you can select the following event logs:

- **Users Event Log.** Displays the event log for all users.
- **Event Log.** Displays the event log for the specified user.



*Figure 62. User event log*

### 7.5.3 Projects and dataset event logs

From the Project window, you can view event logs that list events related to a project, such as adding or removing datasets. In the Projects window, you can select:

- **Projects Event Log.** View an event log for all projects.
- **Event Log.** View the event log for a specific project.

*Figure 63. Project event log*

### 7.5.4    Spectral source event logs

From the Spectral Sources window, you can view event logs that list events related to a specific spectral source, or all of them. This log records all changes to spectral sources, such as adding new spectral sources, starting or stopping acquisition on a Raman Rxn analyzer, or changing batch collection settings in the Raman Analyzer window. In the Spectral Sources window, you can select:

- **Spectral Sources Event Log.** View an event log for all spectral sources.
- **Event Log.** View the event log for a specific spectral source.



*Figure 64. Spectral source event log*

### 7.5.5    Data fields event logs

From the Data Fields window, you can view event logs that list actions related to a specific data field, or all of them. This log collects all changes to data fields, including adding new fields, removing fields, or adding aliases. In the Data Fields window, you can select:

- **Data Fields Event Log.** View an event log for all data fields.
- **Event Log.** View the event log for a specific data field.

*Figure 65. Data fields event log*

# 8       Diagnostics and troubleshooting

## 8.1      Restarting or turning off the analyzer

**To restart or turn off the analyzer:**

1.   From the **Raman Analyzer** window, click **Options**.

     The Analyzer Options dialog appears.
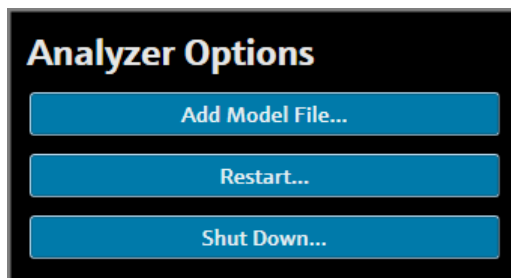
*Figure 66. Analyzer options*

2.   Choose one of the following:

     ▪   Click **Restart** to restart the analyzer.

     ▪   Click **Shut Down** to shut down the analyzer.

3.   Click **OK** on the confirmation dialog.

After a Raman RunTime analyzer has been turned off or reset, restart the Windows Service to connect Raman data library to RunTime. To restart the Windows Service, stop and then start the **Endress+Hauser Raman data library** service using the tray service manager, or restart the Raman data library computer.

## 8.2      Spectra are not being collected

If spectra are acquired using the Raman Analyzer window and the spectra are not added to a dataset, this indicates that the Windows Service has disconnected from the Raman RunTime analyzer and the connection needs to be reestablished.

The Windows Service can disconnect from the Raman RunTime analyzer for various reasons, including:

▪   Shutting down the analyzer for extended periods of time

▪   Changing network settings in the Raman RunTime software

▪   Changing network settings on the computer running Raman data library.

To reconnect the Windows Service connection, stop and then start the **Endress+Hauser Raman data library** service using the tray service manager, or restart the Raman data library computer.

# 9    Support

## 9.1    About

Click **About** in the top ribbon to open the About Raman Data Library window. This window displays the software version and version number, installation ID, and copyright information.



*Figure 67. About window*

## 9.2    Contact information

For technical service, refer to our website (https://endress.com/contact) for the list of local sales channels in your area.

# 10    Copyright information

## 10.1    End-User License Agreement

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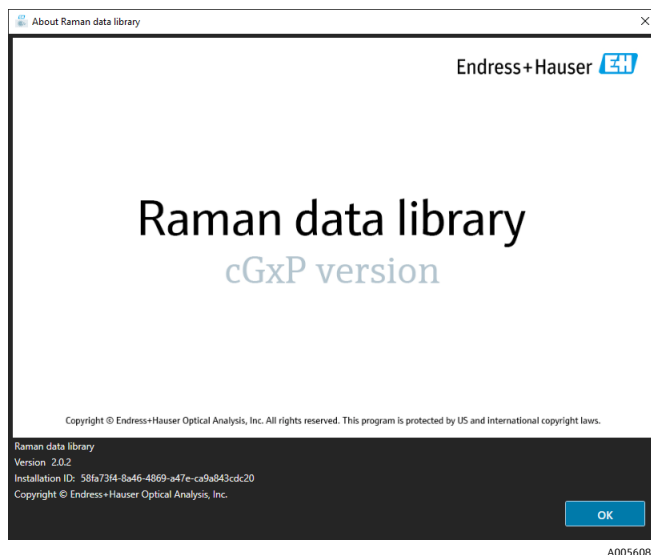
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5.2. No modification of this Agreement shall be binding unless it is in writing and is signed by an authorized representative of the party against whom enforcement of the modification is sought.

5.3. Any notices required or permitted under this Agreement shall be in writing and delivered in person or sent by registered or certified mail, return receipt requested, with proper postage affixed.

5.4. In the event that any of the terms of this Agreement is or becomes or is declared to be invalid or void by any court or tribunal of competent jurisdiction, such term or terms shall be null and void and shall be deemed severed from this Agreement and all the remaining terms of this Agreement shall remain in full force and effect.

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