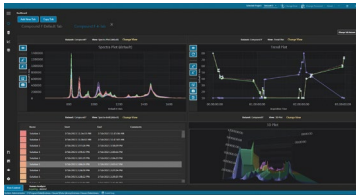# Technical Information

# Raman data library

Spectra storage, organization, analysis, and
multi-analyzer data collection from lab to cGxP



## Application

Endress+Hauser's Raman data library is software designed to organize, read, analyze, and
report on Raman Rxn spectral data. Raman data library complements the Endress+Hauser
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. Users can also export prepared data
for external multivariate modeling. In addition, Raman data library was created for users who
need to collect and store Raman spectra according to FDA 21 CFR part 11 requirements for
traceability during creation and execution of Raman-based analytical models.

## Your benefits

- **Data organization features**: Matches spectra to reference values, data preparation prior
  to chemometric modeling, searchable data storage, data integrity
- **Data analysis features:** Spectra visualization and simple analysis such as peak trending
  and modeling
- **cGxP option:** Meets industry standards for spectral data traceability, storage, and
  archival

Endress+Hauser

People for Process Automation

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# Application

**Graphic visualization of Raman data library's suggested workflow**

Raman data library suggested workflow

Create project → Add spectral sources → Create dataset

Apply pretreatments → Define peaks and regions

Define views and dashboard → Create templates
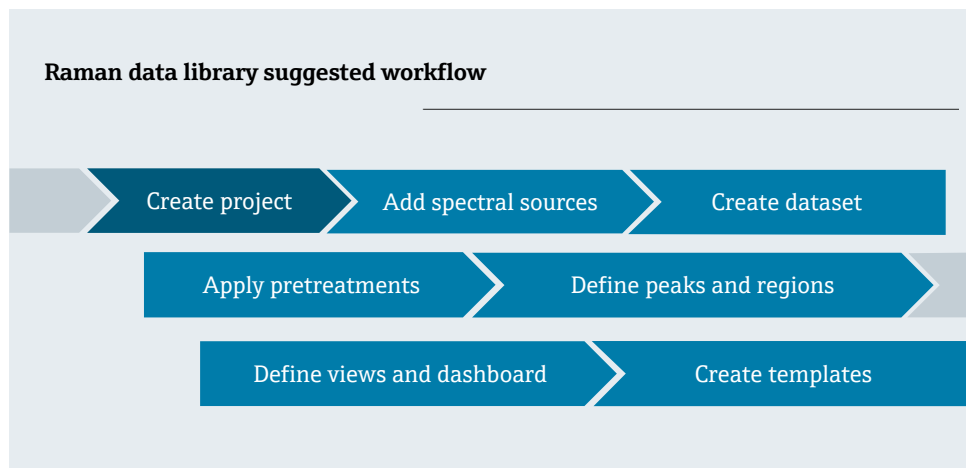
**Use cases**

This software is designed to fit the needs of use cases common to multiple industries:

- Real-time data import from Raman RunTime
- Project-oriented data organization
- Data matching for modeling prep
- Visualize spectral changes
- Peak and region analysis and univariate modeling
- Export to chemometric programs

**cGxP use:** Collect, view, store, retrieve, and archive data per FDA 21 CFR Part 11 requirements:

- User action traceability and data integrity
- View and store data from multiple analyzers and probes
- Data search, retrieval, and (basic) reports for audit support

# Versions

**Raman data library–core version**

### Raman Rxn analyzer control

- The Rxn Control area of Raman data library resembles the user interface for Raman RunTime.
- The Rxn control area interface is responsive to analyzer configuration, differing presentation of single channel, multi-channel, and Hybrid analyzers.
- Multiple analyzers can be connected, monitored, and controlled from one central place.
- Raman data library provides an interface for Raman Runtime, in which Raman Rxn analyzers can be calibrated and verified.
- Analyzer calibration reports can be accessed, and model files can be sent to analyzer.
- The Rxn Control feature facilitates initiation and control of Raman data collection.

### Data collection

- Without any user input, Raman data library can display spectra and model results from Raman RunTime and all its supported predictors.
- Raman data library connects to Raman RunTime via OPC UA.
- Raman data library provides encrypted and searchable data storage and archival.

### Data fields

- Data fields are qualitative and quantitative info tagged to a spectrum.
- For quantitative analysis, the user can specify precision, units, primary method details, etc.
- Aliases can be added to reduce user error for imports, for example, Glucose = glucose.
- Data Field names follow models all the way.

### Pretreatments

- Baseline correction methods, normalization, and other spectral pretreatments can be applied.
- The user defines the sequence of pretreatments.

### Peaks, regions, and peak models

- Peaks can be trended by height, area, or center.
- Peaks can be assigned to Data Fields and modeled.
- Regions can be selected for principal component analysis (PCA) or multivariate curve resolution (MCR) analysis, providing insight into outliers or spectra trends without focusing on specific peaks. This is a "no model" approach to analyzing spectra.

### Views

- Views define the most relevant plots for each user or use case.
- There are many options for plots, even for simple datasets.
- Trend plot options include model predictions from RunTime, Raman data library peak model predictions, measured reference data, and more, for all data fields and peak selections.

### Dashboards

- A dashboard is a collection of plots/views.
- Users can create preferred dashboard tabs that display 1 to 4-plot quadrants.
- The Dashboard is intended to be the main view for routine analysis at-a-glance.

### Templates

- Templates remember all pretreatments, analysis, and view settings and can be applied to new datasets.
- If pretreatments, peak analysis, and views are saved to a template, a user can go straight from dataset creation (new Raman RunTime batch or SPC import) to the Dashboard to view results.

### Dataset analysis

- Users can import spectra and reference data and can analyze the created datasets through a tabbed workflow.
- Analysis can be done in real-time, or data can be exported for post-treatment analysis.

- Datasets can be combined for analysis or modeling within Raman data library, or for export to external multivariate data analysis (MVDA) software.
- Generic exports (.csv and .spc), GRAMS IQ™ (.cfl), and SIMCA® (.usp) are supported.
- All spectra can be exported without pretreatments (default) or with pretreatments.
- Time-based trends are not applicable for all datasets.
- Outliers can be selected from the box and trend plots.

**Multivariate curve resolution (MCR)**

- MCR covers a wide span of algorithms designed for mixture analysis by expressing the original data as an estimate of pure component information.
- Calculated pure component spectra and trends can be displayed within Raman data library.

**Principal component analysis (PCA)**

- PCA is used to reduce the number of variables of a large data set, while preserving as much information as possible.
- In Raman data library, PCA's primary function is for the user to observe trends in datasets that may not be obvious from viewing the spectra plots or individual peak trends. It can also be used to identify and exclude outliers.
- *PCA models cannot be saved to a Raman data library model (for implementation in Raman RunTime), but PCA analysis is saved as part of a dataset template.*

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**Raman data library–cGxP version**

Raman data library can be FDA 21 CFR Part 11 compliant when installed with the cGxP Setup installer and qualified via IQ/OQ (executed by Endress+Hauser) and PQ (executed by 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.

Raman data library allows for storing spectral data in a secure database, performing calculations on the spectral data, and displaying spectral data and its associated metadata.

- All features available in the regular version are available in the cGxP one.
- For the cGxP version, all actions are traceable so sign in, sign out, and user management is required.

To change from Raman data library core to the cGxP version, the program must be reinstalled.

**Role-based user access**

Raman data library cGxP features native user management. An administrator with the Users Manager role can create and manage users, including assigning user roles. User credential authentication can be tied into Microsoft Active Directory.

A user can be given multiple roles, and the user-role functionality offers flexibility to implement site-based user groups.

| Role | Actions Allowed |
|------|-----------------|
| Data Remover | Remove datasets, spectra, data fields, and projects |
| 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> |

| Role | Actions Allowed |
|---|---|
| Projects Manager | Add and edit projects |
| Users Manager | Add, edit, and disable users |
| Analyzer Calibrator | Calibrate a Raman Rxn analyzer |
| Analyzer Verifier | Verify a Raman Rxn analyzer |
| Analyzer Operator | Start, stop, and pause dataset acquisitions |
| 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> |

# System requirements

Raman data library is a 64-bit Microsoft Windows program that runs on Microsoft Windows™ 10 Professional.

**Raman data library–core**

**Operating system**

Microsoft Windows 10 (Professional 64-bit)

**Hardware**

- Processor type: Intel Core i5 or equivalent processor
- Main memory (RAM): 16 GB
- Hard disk capacity: 10 GB or higher, depending on database size
- Screen size (desktops): 24" or more with a resolution of 1920 x 1080 or greater, and appropriate display scaling settings
- Screen size (laptops): 13" or more with a resolution of 1920 x 1080 or greater, and appropriate display scaling settings

Microsoft .NET Framework version 4.7.2 is also required.

**Raman data library–cGxP version**

**Operating system**

Microsoft Windows 10 (Professional 64-bit)

**Hardware**

- Processor type: Intel Core i5 or equivalent processor
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# Specifications

**Communication**

Communication to Raman RunTime is through OPC UA. HTTPS protocol is also used to transfer certain files between Raman RunTime and Raman data library, such as model files.

**Database**

Raman data library uses a secure embedded database. The database SQLite, provided by a third party, provides a full-featured relational database management system (RDBMS).

# Installation

**Installation**

Administrator privileges are needed for installation and configuration of Raman data library.

# Supplementary documentation

**Quick start**

KA01717C Raman data library Brief Operating Instructions

**Operating instructions**

BA02367C Raman data library User Operating Instructions

BA02349C Raman data library Administrator Operating Instructions

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