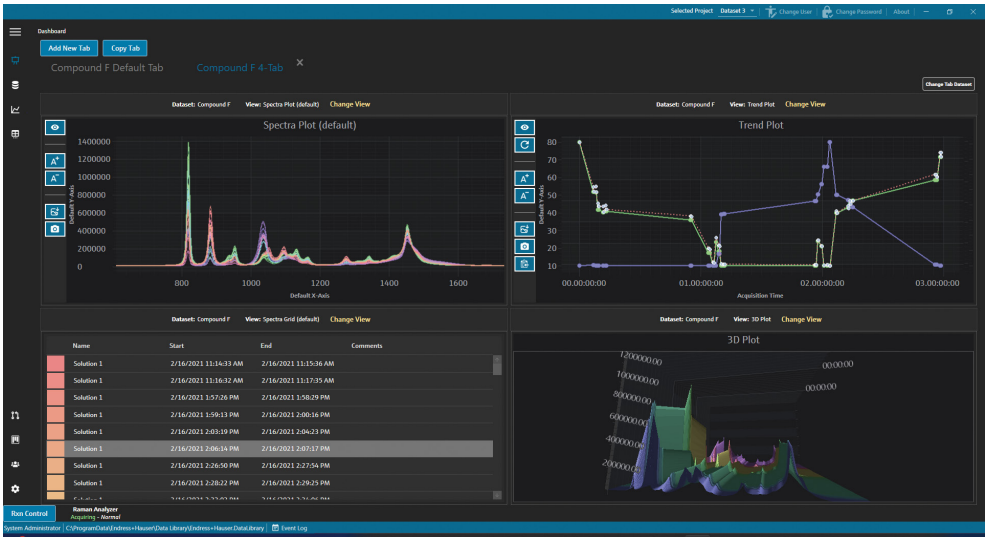
Raman data library

Faster time to market with increased insight, productivity, and data integrity

Benefits at a glance

- **Intuitive interface and workflow** facilitates quick user adoption
- **Spectral visualization and trend plots** provide a window into your process
- **Immediate process feedback** enables no-model analysis for rapid response
- **Customizable templates** improve productivity and reduce user error
- **Multi-analyzer control** standardizes data from collection through analysis
- **User management and audit trails** streamline cGxP validation, reducing costs and time



Raman data library dashboard

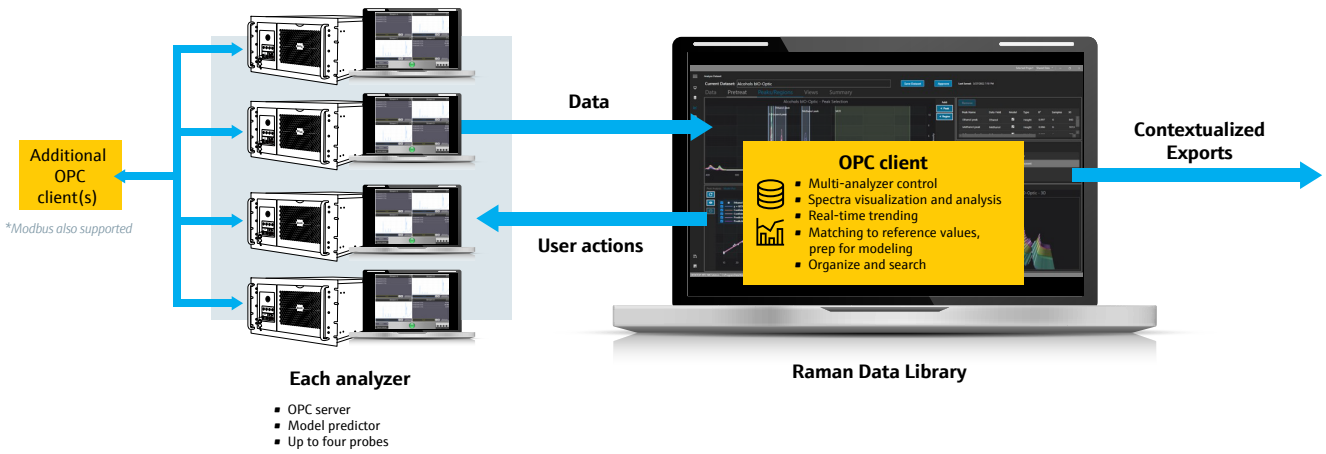
Raman data library is a unique software program designed to organize and visualize spectral data tailored to your specific application and site requirements. Multi-analyzer communication with a central, searchable data repository enables easy data retrieval. Customizable templates, dashboards, auto-tagging, and project-oriented features significantly reduce time and user error in your Raman workflow.

From basic peak and region trending to quantitative peak-based modeling, Raman data library offers a simplified workflow for analysis of Raman spectra. For more advanced applications, there are export features designed specifically for handing spectral datasets over to data scientists and external modeling platforms.

The cGxP version of Raman data library enables compliance with 21 CFR part 11 guidelines and ALCOA+ principles. Customizable user privileges and user management through Windows Active Directory align with IT preferences. Encryption of the database and industry standard communication protocols add another layer of security. The cGxP version also carries the option of extra documentation to support system qualification. Raman data library's simplified implementation of data-oriented regulatory requirements streamlines moving Raman from the lab into cGxP.

Endress+Hauser

People for Process Automation



System overview of Raman data library – core implementation

Raman data library – core

Ensuring seamless transitions across analyzers and sites, from laboratory to process environments

Raman data library offers a streamlined, affordable, and scalable solution for spectral data visualization and analysis. It includes automation-ready features for organizing and storing Raman spectra along with complementary qualitative and quantitative data. Raman data library can connect to multiple Endress+Hauser Raman analyzers, enable cross-site collaboration, provide impromptu pre-processing and analysis, and contextualize exports for advanced modeling.

Multi-analyzer control

Up to four Raman Rxn analyzers can be connected to Raman data library, supporting monitoring, visualization, and collection from up to 16 Raman probes at once.

Data organization

Raman data library auto-matches Raman spectra to imported reference values, tags spectra for categorization, prepares datasets for univariate (e.g., peak area) or multivariate (e.g., PLS) modeling, and stores data for searchable retrieval, all while ensuring data integrity.

Data analysis

Datasets are analyzed through a structured, tabbed workflow. Key steps include aligning spectra to reference data, applying pretreatments, selecting significant peaks and regions, removing outliers, and correlating variations in Raman spectra to sample or process changes. Analysis can be conducted in real time or saved for future use.

Data visualization

Spectra viewing options are flexible and customizable–2D, 3D, raw, pre-processed, zoomed in or out, annotated, and color coordinated. Plots of imported reference data, peak trends, and model predictions can also be tailored to the user's preference. For example, trend plot selections include:

- Peak area, height, and center profiles
- Measured reference data (e.g., sample concentration)
- Univariate and multivariate model predictions

Analyzer control with real-time display enables swift, actionable insights. Trend plots facilitate proactive measures, while data organization and cleaning ensure data reliability. These tools collectively accelerate and simplify transition from lab-to-process, optimizing efficiency and reducing errors.

Highlighted features

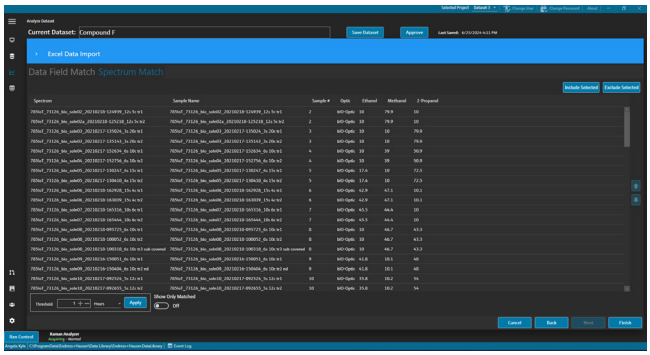
- Data visualization in real time
- Date/time or tag searching for data retrieval
- Templates for pre-structured data
- Standard communication protocols for remote control of analyzers
- Multi-analyzer communication
- Data encryption
- Multi-site collaboration and monitoring through network share (on licensed PCs)

Raman data analysis features

Guided workflows, automated data matching, rapid trending, efficient templates, and datasets prepared for external analysis

Matching spectra to reference data

Raman data library's spectrum match workflow enables the alignment of selected spectra to qualitative and quantitative information imported from an Excel file. Quantitative data can be specified by the measurement units, primary method type, ID (e.g., serial number), and other details. Qualitative data to categorize spectra can be anything from tags (e.g., batch ID) to user comments.



Spectrum matching

Peak and region analysis

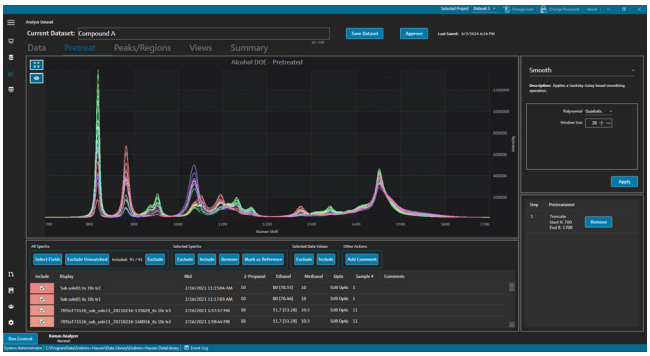
Peaks can be trended by height, area, or center simply by selecting points on a spectral plot. If quantitative data values have been imported, then peak changes can be correlated to these values to create predictive models.

Regions can be selected for multivariate curve resolution (MCR) or principle component analysis (PCA) to spot outliers and learn about spectra trends without focusing on specific peaks. This provides a no-model approach to analyzing spectra, perfect for new applications and users new to spectroscopy.

Selecting peaks and viewing trends

Data pretreatments

To prepare Raman spectra for analysis and modeling, baseline correction methods, normalization, smoothing, and other spectral pretreatments can be applied. The user can define the type and sequence of pretreatments.



Applying pretreatments to data before modeling

Templates

Templates simplify dataset creation and routine analysis. They contain spectral collection settings, pretreatments, selected data fields, peak and region analyses, and dashboard viewing options. Apply them for immediate data interpretation when creating a new dataset.

Exporting for additional analysis or model prediction

Datasets can be combined for analysis and modeling within Raman data library, or for export to external programs. To export a peak model created in Raman data library, a custom file format is used (.dlm) which is compatible with Raman RunTime v6.4+.

Exported datasets contain all selected spectra and data fields (qualitative/quantitative data and spectrum diagnostics). Supported export formats include:

- SIMCA® (.usp)
- GRAMS IQ™ (.cfl)
- CSV (.csv & .spc)—Generic export compatible with standard chemometric/MVDA programs


785IoT_73126_bio_soln17_20210216-160317_6s 10c tr1
785IoT_73126_bio_soln15_20210216-163258_6s 10c tr1
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Default Y-Axis
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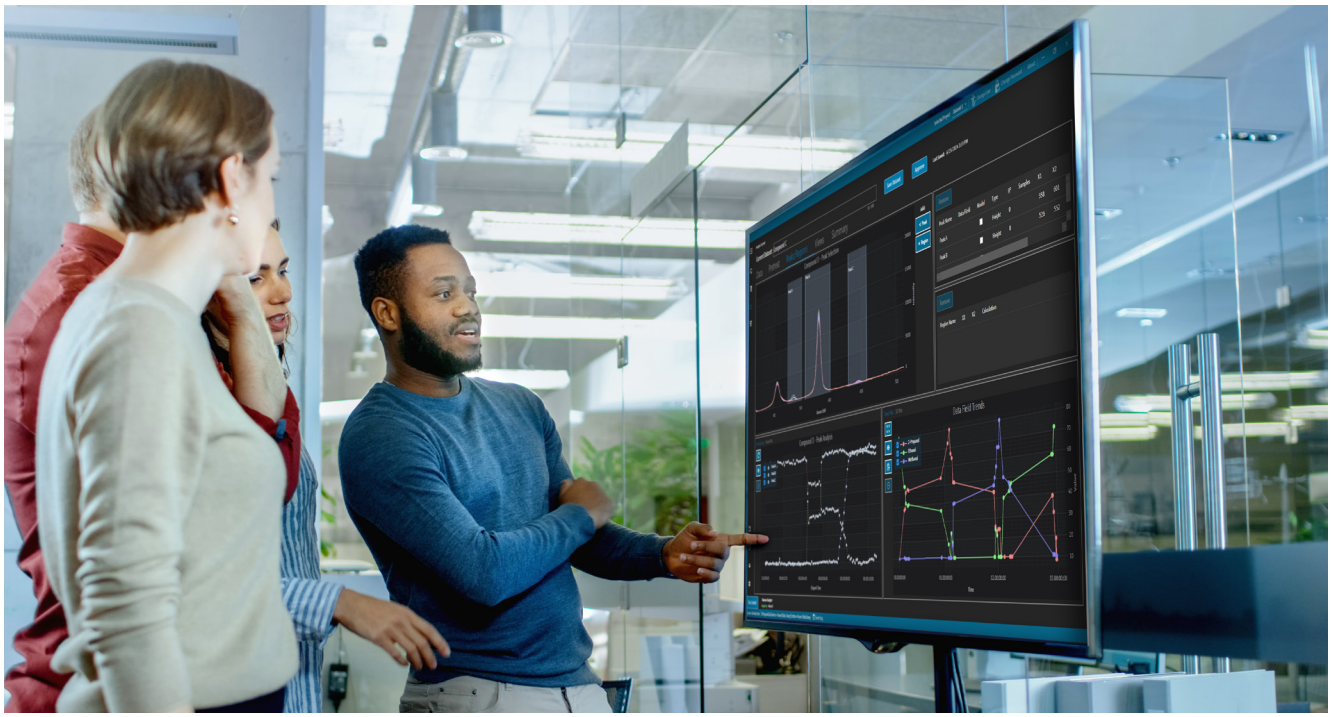
Data aggregation and visualization

Multi-analyzer control and spectra management with customizable views



Flexible dashboard display

The Raman data library dashboard is a collection of plots customized to a user's preference. Deep dive into analysis of a single dataset or display information from multiple datasets, probes, and analyzers side-by-side.

The dashboard is intended to be the main area for routine analysis. When pretreatments, peak analysis, and plot preferences (called views) are saved to a template, a user can go straight from spectra collection (or import) to viewing results in the Raman data library dashboard. From the dashboard:

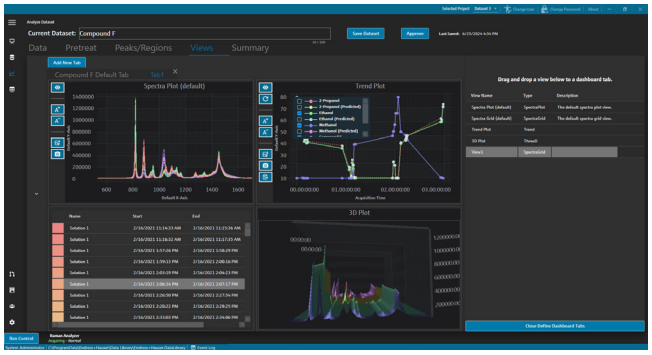
- Users can create preferred tabs that display up to four plot quadrants.
- These tabs launch on start-up and provide immediate feedback, aiding in reliable decision-making.
- Plots update in real-time as new spectra are collected.

Raman Rxn analyzer control

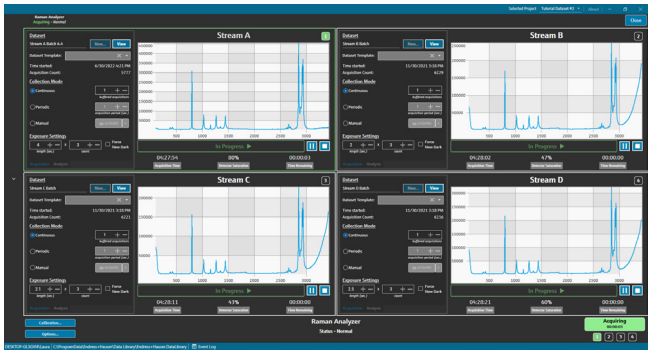
The Rxn control area of Raman data library resembles the Raman RunTime's user interface for a familiar feel. Raman Rxn analyzers can be calibrated, verified, started, paused, stopped, and rebooted directly from this area.

Raman data library connects to Raman RunTime (v6.4+) via OPC UA. Through this connection, Raman data library does the following:

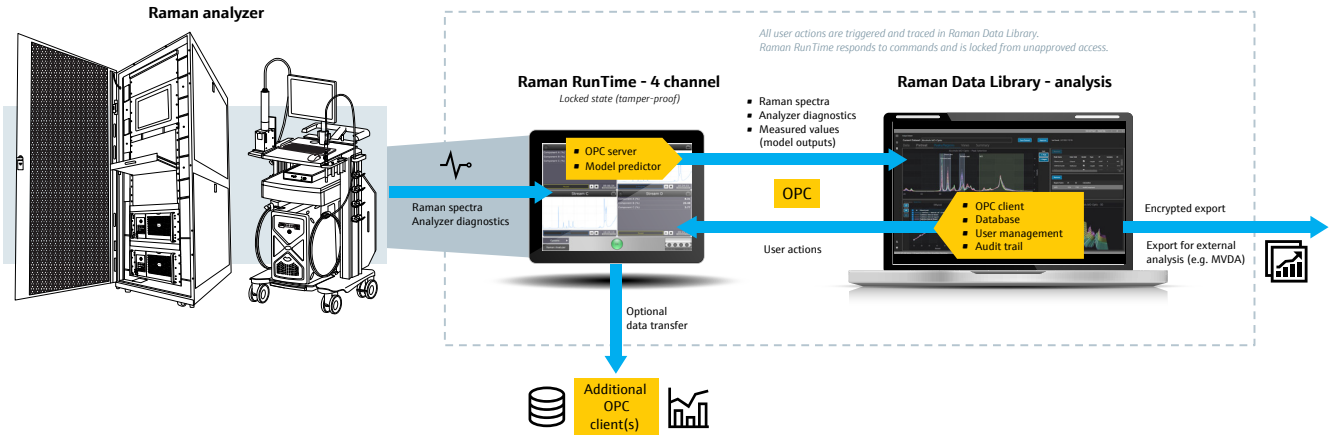
- Transfers model and probe (intensity) calibration files to Raman RunTime
- Defines or changes collection settings and initiates Raman collection start, stop, and pause
- Receives spectra, model outputs, & analyzer diagnostics
- Links spectra to analysis and dashboard areas (in real time or post-process)
- Performs data storage and archival



Defining the Raman data library dashboard



Raman Rxn analyzer control in Raman data library



System overview of Raman data library cGxP version implementation

FDA 21 CFR part 11 compliance features

Centralized and affordable compliance supporting easy Raman scale up from the lab to cGxP

The cGxP version of Raman data library was developed to streamline compliance with the latest ALCOA+ principles and Good Automated Manufacturing Practice (GAMP) guidelines. This version features the ability to collect and store multi-analyzer data according to FDA 21 CFR Part 11 requirements, as well as integration with Windows Active Directory to meet standard IT site requirements.

Raman data library's user administration permits only users logged in with a unique user name and password to enter data in accordance with their access authorization and role. User actions and analyzer events are date and time stamped and recorded in the event log.

Raman data library also offers the following security features to further increase data integrity and align with site-specific IT protocols. Most of these security features are configurable with administrator-level privileges:

- Password length and expiration rules
- User management with customizable user privilege settings – from data collection through analysis actions
- User-lockout after login failures
- Auto-logout after inactivity
- Change control for user entry edits

For Raman system installations in regulated environments, this version of Raman data library offers the option of receiving support documentation including a URS, compliance questionnaire, ER/ES assessment, and IQ/OQ test report. In addition, IQ/OQ/re-OQ and technical support services are available worldwide.

The cGxP version of Raman data library facilitates 21 CFR part 11 compliance in a cost-effective manner. It serves as a gateway for Raman transition from lab to production and standardizes data across sites, without the need to invest in a high-cost, complex spectra-compatible software infrastructure. These powerful features enhance a Raman system investment, maximizing the value of your Raman implementation.

Highlighted features, cGxP version

- Enables 21 CFR Part 11 compliance
- Audit trail of events and user actions
- User management through Windows Active Directory
- Customizable user privilege settings
- Electronic records and sign-offs
- Multi-analyzer communication
- Data encryption

Related product pages: Raman Rxn2 analyzer | Raman Rxn4 analyzer

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