Enhance productivity and ensure data integrity

Customizable, user-friendly spectral analysis with Raman data library software

Raman data library

Simplifying Raman spectral data analysis

Raman data library is the perfect go-to software for organizing and analyzing Raman spectral data with ease. Its intuitive interface and streamlined workflow make it simple for users of all expertise levels to visualize, analyze, and store spectral data.

Scalable and automation-ready, Raman data library is an affordable way to maximize the power of Raman spectroscopy without having to invest in expensive external packages or develop customized, complex data handling systems.

The software is available in two versions:

- **Core version:** Ideal for general use in a wide range of applications
- **cGxP version:** Advanced functionality for meeting industry standards (FDA 21 CFR Part 11) for spectral data traceability, storage, and archival
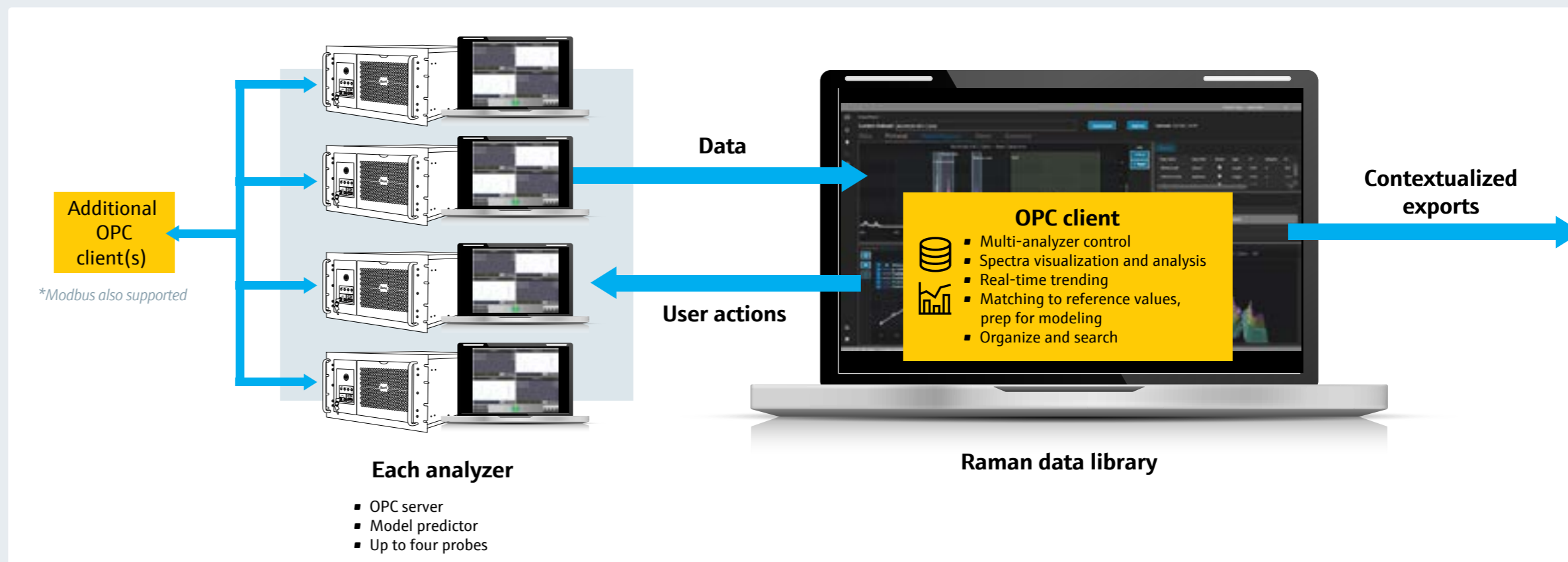
Raman data library – core version

An essential tool for spectral data management

The core version of Raman data library allows users to easily view, organize, analyze, and model Raman data for application development and routine monitoring in laboratory or process environments.

Raman data library enables centralized, remote data collection and control of multiple Raman analyzers across sites, while maintaining data integrity. This core software version offers simplified workflows for spectral interpretation, peak-based trending or modeling, or export for multivariate analysis.

Key features:

- Automated reference data matching
- Data visualization in real time
- Date/time or tag searching for data retrieval
- Templates for pre-structured data
- Multi-site collaboration and monitoring through network share (on licensed PCs)
- Streamlined modeling workflow

Additional OPC client(s)
Modbus also supported

Data

User actions

Each analyzer
- OPC server
- Model predictor
- Up to four probes

OPC client
- Multi-analyzer control
- Spectra visualization and analysis
- Real-time trending
- Matching to reference values, prep for modeling
- Organize and search

Raman data library

Contextualized exports

System overview of Raman data library – core implementation

Your challenge
Task: Real-time chemical composition measurement with efficient spectral data management from lab to process

Solution: The core software version features:

- Data collection, viewing, storing, retrieval, and archiving
- Real-time data import from Raman RunTime
- Process trending and visualization
- Project-oriented data organization
- Data matching for modeling prep
- Peak and region analysis with quantitative peak modeling
- Contextualized exports to chemometric programs

Our answer
The **core version of Raman data library** provides analyzer control with real-time display, providing you with swift, actionable insights. Trend plots facilitate proactive measures, while data organization and cleaning ensure data reliability. These tools collectively accelerate and simplify the transition from lab to process, optimizing efficiency and reducing errors. The program offers an affordable alternative to external packages or in-house data handling systems, reducing ongoing IT infrastructure development and maintenance expenses.
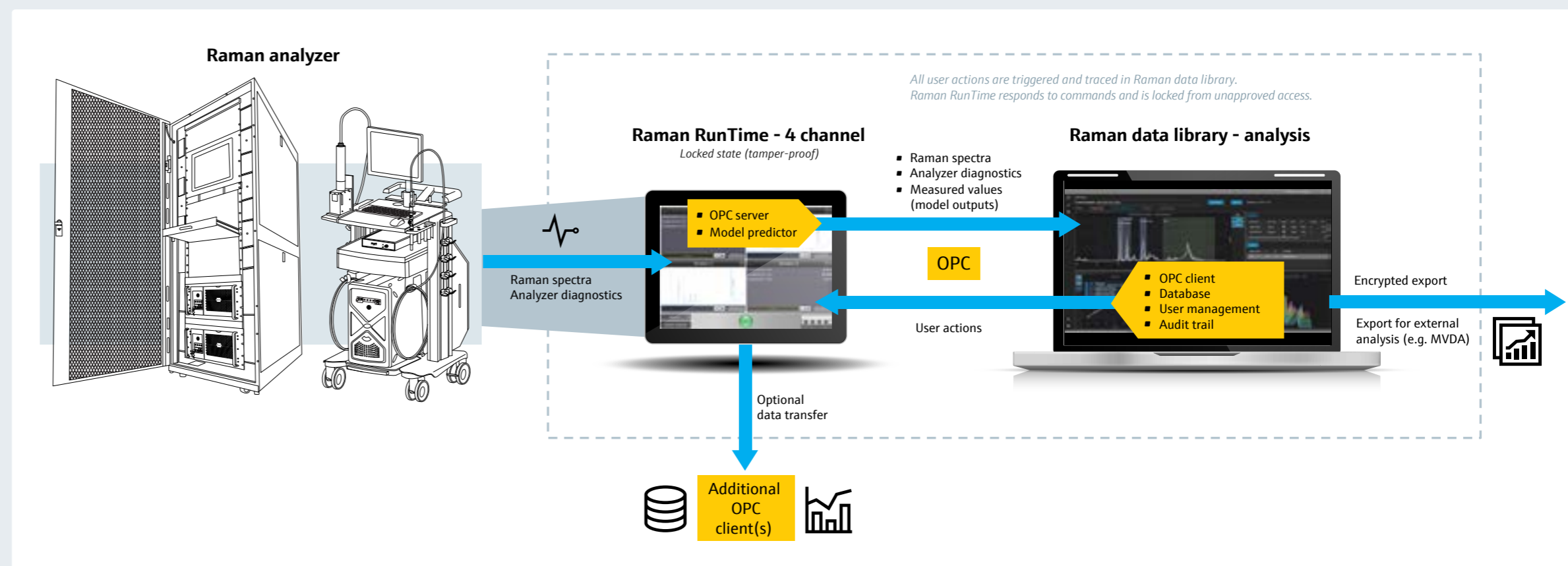
Raman data library – cGxP version

Easy regulatory compliance for Raman scale up from lab to cGxP

The cGxP version of Raman data library offers the same benefits as our core version, with added features to support cGxP compliance.

Raman data library's cGxP implementation provides expanded user management and spectral data traceability, storage, and archiving. In doing so, it ensures compliance with 21 CFR Part 11 guidelines and ALCOA+ principles. By embedding data-oriented regulatory requirements, the cGxP version of Raman data library simplifies the transition of Raman spectroscopy from lab to production environments.

cGxP version highlights:

- 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
- Optional documentation support (URS, ER/ES assessment, IQ/OQ test report, etc.)

System overview of Raman data library – cGxP implementation

Your challenge
Task: Real-time chemical composition measurement from lab to cGxP in compliance with 21 CFR Part 11 guidelines

Solution: In addition to its core features, the cGxP software version offers:

- Spectral data traceability
- User management
- Electronic records and sign-offs
- Audit trail
- Enhanced security features

Our answer
The **cGxP version of Raman data library** facilitates 21 CFR part 11 compliance in a cost-effective manner with spectral data traceability, user management, electronic record keeping, electronic signatures, and audit trail capabilities. Furthermore, a connection to a central user administration (e.g., Microsoft Active Directory) is possible. It serves as a gateway for transitioning Raman spectroscopy from lab to production, standardizing data across sites without the need for an expensive, complex spectra-compatible software infrastructure. The cGxP version enhances your Raman system investment, maximizing the value of your Raman implementation.

Benefits at a glance

Speed time to market with greater insight, data integrity, and productivity

The right tools make the complexity of interpreting Raman data easy. Raman data library was developed for just that purpose — to simplify how users organize and analyze their Raman data.

Raman data library allows scientists and engineers to visualize composition changes in real time for faster insights and better decision-making. Its user-friendly interface, efficient multi-analyzer control, and customizable workflows speed up routine analysis and reduce user error which accelerates time to market.

The software ensures compliance with regulatory standards and maintains data integrity while enabling seamless Raman scale up from the lab to full-scale manufacturing.

Seamless scalability and compliance
Centralized and affordable regulation compliance supports smooth Raman scale up from lab to process

Faster process development
Peak-based data trending saves model development time, effort, and expertise

Rapid process insights
Real-time process insights enable better data-driven decisions

Enhanced data security
Increased data integrity and encryption complies with industry standard communication protocols

Customizable templates
Pre-structured data templates improve productivity and reduce user error

Efficient multi-analyzer control
Standardized data collection from multiple analyzers across sites enables more efficient analysis

Lower IT infrastructure and maintenance costs
Scalable, automation-ready capabilities reduce the need for costly external software or custom systems

Quick user adoption
Streamlined user interface and workflows reduce user learning curves

Industry focus

Simplifying the user experience across industry applications

Tailored to specific applications and site requirements, Raman data library helps users organize, visualize, and analyze their spectral data efficiently with a focus on providing a simplified overall user experience.

Whether new to Raman spectroscopy or an experienced user seeking a scalable solution, Raman data library is well-suited for use in a wide variety of applications.

For regulated markets, it ensures compliance with data integrity standards, making it particularly beneficial for lab and process environments in the Life Sciences, Food & Beverage, and Chemical industries.

Life Sciences industry

Simplify Raman analysis for fast market entry, smooth scale up, and higher yields

Raman spectroscopy is widely used to monitor, adapt, and control Life Science processes. For scientists and process engineers who wish to simplify spectral data analysis, organization, and storage, Raman data library software is the answer.

By delivering rapid process insights, streamlining workflows, reducing human error, and enabling easy scale up of Raman data from lab to commercial scale, this software helps Life Science manufacturers get to market faster and achieve higher yields.

Raman data library also aligns with Industry 4.0 and ensures regulation compliance without the complexity and high investment of developing internal systems or a full Process Analytical Technology (PAT) platform.

It is available in both a core version and a cGxP version with expanded capabilities to facilitate 21 CFR Part 11 compliance.

Food & Beverage industry

Fully leverage Raman process insights to
maximize product quality and productivity

In the Food & Beverage industry, Raman data library enables a streamlined adoption of Raman spectroscopy as a tool to quickly build process knowledge and speed up process development in a laboratory or scale-up environment.

Raman data library's intuitive interface and robust analytical capabilities empower users to conduct precise and reliable spectral analysis. This aids in speeding process development and identifying highly specific markers of product quality for inline control. The quicker implementation of Raman spectroscopy in process development ensures more efficient processes and offers a pathway toward inline quality measurements.

Raman data library serves as a comprehensive software solution, facilitating both laboratory and process implementation of Raman spectroscopy. It ensures seamless scalability, making it easier for Food & Beverage manufacturers to adapt to varying production demands and regulatory requirements.

Chemical industry

Harness the power of Raman analysis for
enhanced safety and optimal reaction control

Inline composition measurements using Raman spectroscopy is
a proven way to achieve product quality and productivity goals
in batch reactors for a variety of chemical industry applications.
Raman data library software offers peak-based trending for
swift inline implementation and supports industry-standard
communication protocols for remote analyzer control.

Its simplified modeling workflow facilitates the rapid
deployment of inline Raman spectroscopy, enabling the
monitoring and control of multiple components within a batch
reactor. This makes it an essential tool for both analytical
development and process engineers.

Raman data library helps chemical manufacturers boost plant
safety and performance by quickly realizing the benefits of
inline Raman spectroscopy for optimal reaction control.

Raman spectroscopy

Illuminating molecular secrets

Technology overview

Utilizing visible or near-infrared light, Raman spectroscopy reveals intricate details about molecular vibrations. As light interacts with these vibrations, it undergoes inelastic scattering, resulting in a unique "molecular fingerprint." This powerful technique enables identification, quantification, and monitoring of specific chemistries.

Raman spectroscopy, traditionally used in laboratory settings, has now become a crucial process analytical technology (PAT) solution in Life Sciences, Food & Beverage, and Chemical industries for process development and commercial manufacturing.

Here's why:

- **Real-time measurement** – Raman provides real-time, *in situ* measurements during various processing operations.
- **Insensitivity to water** – unlike other techniques, Raman measurements remain accurate even in aqueous environments, making it well suited for a wide range of process applications.
- **Specificity** – Raman can distinguish between different molecules, even those with similar structures, enabling precise analysis of complex mixtures in processes.
- **Inline sampling** – directly inserted into bioreactors or flow paths, a single probe can simultaneously measure multiple parameters and quality indicators without disrupting the process.

Raman technology illustrated

- Laser light of specific wavelength interacts with molecules which causes scattering
- 1 out of 10^8 photons is frequency-shifted due to specific energy transfer (Raman shift)
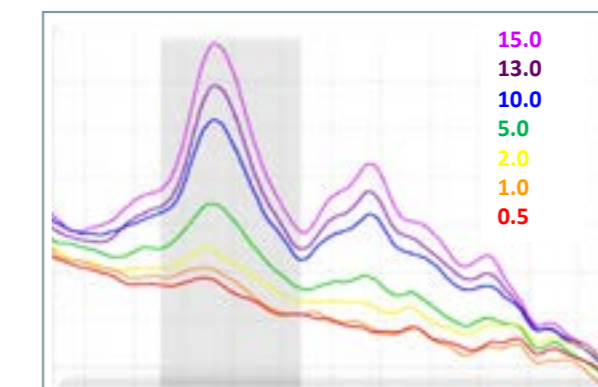- Result: specific photons allow identification and quantification of materials (solvent, products, substrate)
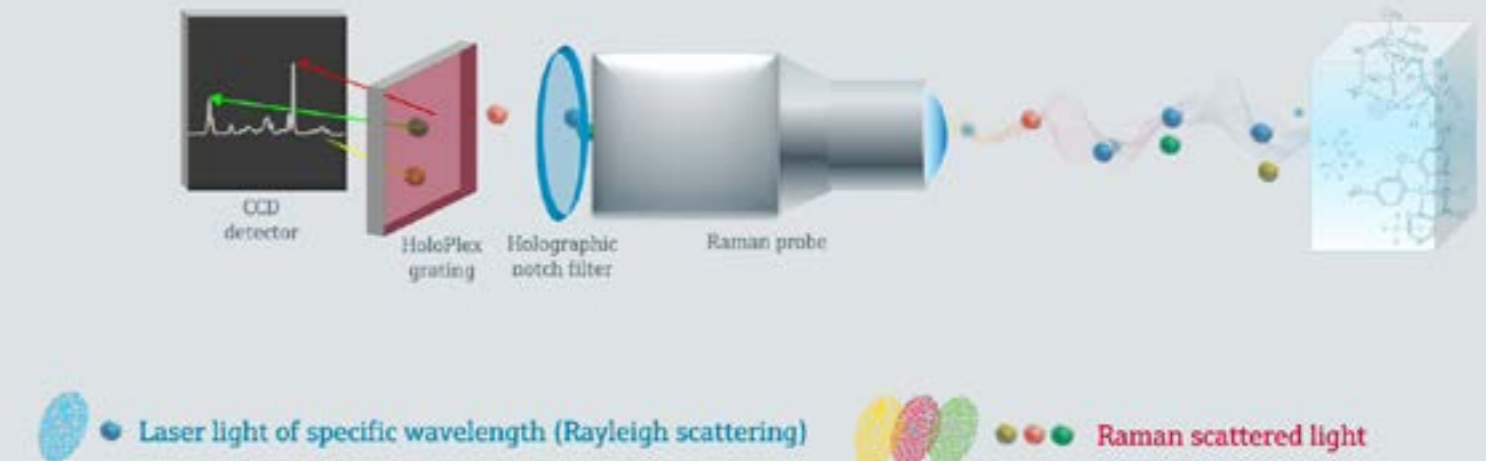
The collected light is interpreted as a spectrum by the camera, creating a "molecular fingerprint" of the material being sampled.

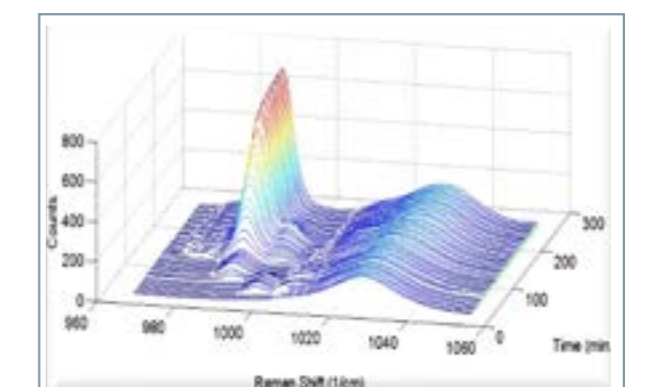## Raman spectra from a lab sample or process can tell us…

What is it?
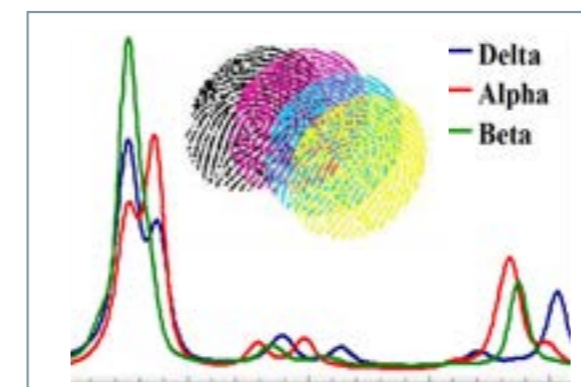
How much?

Has it changed?

Technical data

Prerequisites for installing Raman data library

Raman data library complements the embedded Raman RunTime software in Endress+Hauser's Raman Rxn2 and Rxn4 analyzers. This vital link expands capabilities for spectral storage, organization, analysis, and multi-analyzer data collection from lab to process.

Whether implementing the core version or cGxP version of Raman data library, users should note the system requirements needed for installation.

Operating systems	▪ Microsoft Windows 10 (Professional 64-bit)
Processor type	▪ Intel Core i5 or equivalent processor
Main memory	▪ 16GB
Hard-disk capacity	▪ Disk space needed: 10 GB, depending on database size
Monitor resolution, display	▪ Screen size: 24" or more with a resolution of 1920 x 1080 or greater (desktops) ▪ Screen size: 13" or more with a resolution of 1920 x 1080 or greater (laptops) ▪ Display aspect ratio of 100%
Input	▪ Data import, SPC from Raman RunTime or legacy software, or OPC-UA from Raman RunTime
Output	▪ Raman data library has two-way communication with Raman RunTime (both input and output)
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).
Registered Trademarks	▪ Microsoft ▪ Windows ▪ All other brand and product names are trademarks or registered trademarks of the companies and organizations in question.

Why partner with Endress+Hauser?

30+ years of analysis innovation and customer success

One source, infinite precision
Imagine a world where all your crucial process parameters are measured and analyzed by one reliable source, bringing efficiency and precision right to your fingertips. Your search ends with Endress+Hauser. We do not just offer instrumentation; we provide solutions that meet your unique application needs, optimized for your installation environment.

Unparalleled expertise
For over three decades, we have partnered with companies to empower them to automate and optimize their processes. Our collaboration with industry leaders in Raman technology has honed our expertise, making us the most trusted ally in the analysis arena.

Tailored innovation
Our complete Raman system portfolio — including Raman analyzers, probes, and optics — is engineered to meet the rigorous demands of the industrial landscape.

Seamless scalability
Using standardized instrumentation ensures that your product's transition from lab discovery to commercial manufacturing will go smoothly. Our hardware and software were designed for lab to process — meaning all models, methods, and technology can scale easily without measurement inconsistency or quality risk.

Global support, local excellence
Endress+Hauser offerings come with the reassurance of decades of proven performance in the field. Our reliable world-class devices are also backed by a global network of process automation service and support experts.

People for Process Automation

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