



X-RAY DIFFRACTION

DIFFRAC.EVA V8

What's New, Why It Matters

Software Feature Overview

EVA 8 is a major step forward in XRD data evaluation, extending EVA from a powerful Search/Match tool into a more iterative, automated, and high-throughput analysis environment. The release focuses on three strategic themes:

- **Deeper insight into complex diffraction patterns** through iterative refinement and residual analysis
- **Higher productivity** via batch processing, workflow automation, and improved visualization of large datasets
- **Stronger integration** with the DIFFRAC.SUITE ecosystem (TOPAS, BBE, MEASUREMENT CENTER, XRD ASSISTANT)

This document summarizes the key new capabilities in EVA 8, explains typical use cases, and highlights the concrete benefits for routine users, application specialists, and advanced analysts.

This release elevates EVA into a more iterative, automated, and scalable analysis platform. Key benefits at a glance are

- Faster and more reliable phase identification in complex samples
- Efficient batch refinement and trend analysis across large datasets
- Improved PDF and local structure interpretation
- Stronger automation for QC and high-throughput environments
- Seamless integration with TOPAS, BBE, measurement software, and XRD ASSISTANT

EVA 8 delivers immediate value for routine users while offering powerful new tools for application specialists and advanced analysts—making it a compelling upgrade for both existing customers and new installations

Trust in Phase ID - Profile Fit Residual Search (PFRS)

The headline feature of EVA 8 is **Profile Fit Residual Search (PFRS)**. PFRS extends the classical Search/Match workflow by optionally introducing an **iterative loop between phase identification and profile fitting**. After an initial Search/Match step, EVA automatically performs a profile fit on the selected phases and automatically re-searches unexplained residual regions. Newly identified phases are added, visually distinguished, and may be refitted for preceding residual analysis. This process continues until the measured pattern is sufficiently explained.

Why it matters

- Enables incremental phase identification in **complex or multiphase mixtures**
- Reduces manual trial-and-error when residual peaks remain after an initial match
- Makes EVA more effective for real-world samples with overlapping reflections

Typical use cases

- Phase identification in **strongly overlapping patterns**
- Incremental discovery of minor or trace phases
- Teaching and training scenarios, illustrating the impact of fit models on phase ID

Advanced manual refinement within PFRS

If the automatic fit does not fully describe the data, users can seamlessly switch from the Search tool to the Fit tool at any stage:

- Change the background and profile functions to better represent instrument and sample effects
- Apply preferred orientation corrections (e.g. Pawley, March–Dollase or spherical harmonics)
- Add spectral impurities to the source emission profile

After manual refinement, the PFRS workflow can be resumed, using the improved fit model to re-evaluate residuals. This hybrid of automation and expert intervention is especially powerful for challenging datasets where subtle instrumental or structural effects are found at the same order of intensity as those from minor phase contributions.

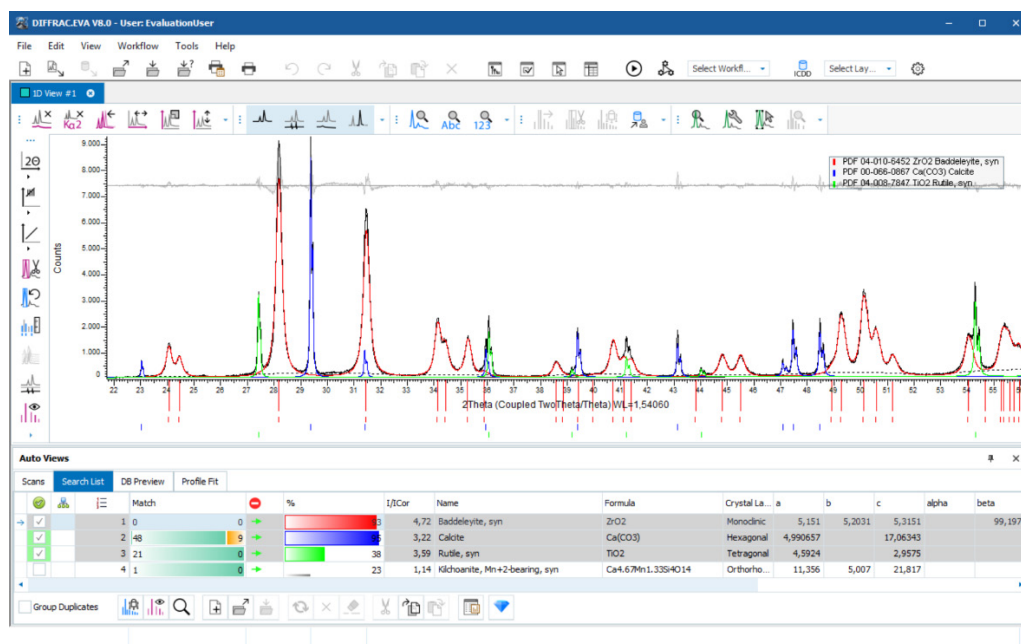


Figure 1

PFRS representation of the profile fit of three phases that were identified and selected in a first pass of an automated search.

Understanding - Atom Pair Histogram Tool for PDF Analysis

A new **Atom Pair Histogram Tool** has been added to the PDF Processing workflow. It provides monoatomic and diatomic pair histograms up to 5 Å, derived from structural data during search-database compilation.

The tool supports interpretation of short-range order features and assists in understanding experimental PDF curves. Interatomic distances are retrieved using chemical filters, conceptually aligned with Phase ID workflows. This new tool

- Improves interpretability of **local structure information**
- Bridges structural databases and experimental PDF data
- Adds educational and explanatory value to PDF analysis

Typical use cases are

- Analysis of disordered, non- or nano-crystalline materials
- Teaching short-range order concepts
- Supporting interpretation of experimental PDF results

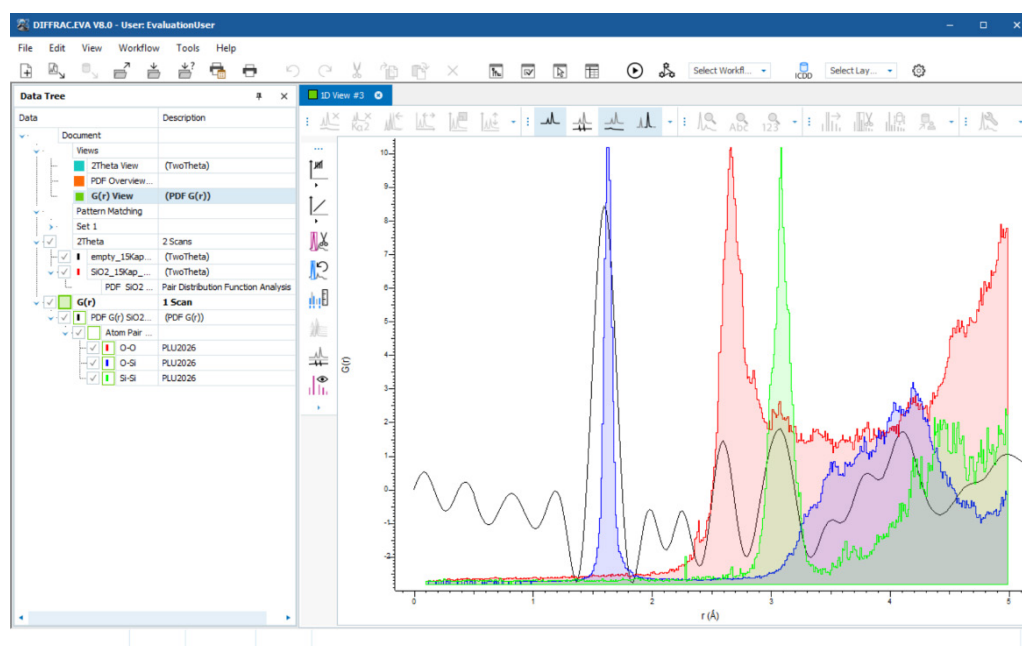


Figure 2

Experimental Pair Distribution Function $G(r)$ of amorphous silica, SiO₂, shown in black. The colored histogram curves explain the first three main peaks in the PDF as originating from Si—O, O—O and Si—Si atom pairs indicating a typical tetrahedral short range order of interlinked building blocks in the silica glass.

Effectivity - Visualization and Evaluation for Scan Lists

List Processing

EVA 8 introduces **Profile Fit for Scan Lists**, enabling a single refinement model to be applied consistently across large series of scans. A defined fit setup can be reused over entire scan lists, with results exported as CSV files for further analysis. Parameter iteration across comparable scans accelerates convergence while maintaining consistency. This

- Dramatically reduces effort for large datasets
- Ensures consistent refinement strategies across scan series
- Facilitates detection of anomalies and trends

Typical use cases comprise

- Phase transformations in non-ambient or operando experiments (peak splitting, peak emergence)
- Monitoring phase formation or decomposition
- Tracking lattice parameter changes versus temperature, time, or other external parameters
- Reproducibility and repeatability studies

3D View

EVA 8 introduces a new **3D View** for scan lists, rendering pseudo-3D intensity maps. With the X-axis the usual scan direction, the Y-axis can represent scan index or metadata such as temperature or time. Color palettes shareable amongst 2D and 3D views ensure a consistent representation is achieved for large datasets. The 3D View allows for

- Rapid visual identification of trends, transitions, and anomalies
- Intuitive overview of complex operando or in-situ experiments
- Improved communication of results

Typical use cases

- Non-ambient experiments
- Time-resolved studies
- Screening large measurement series

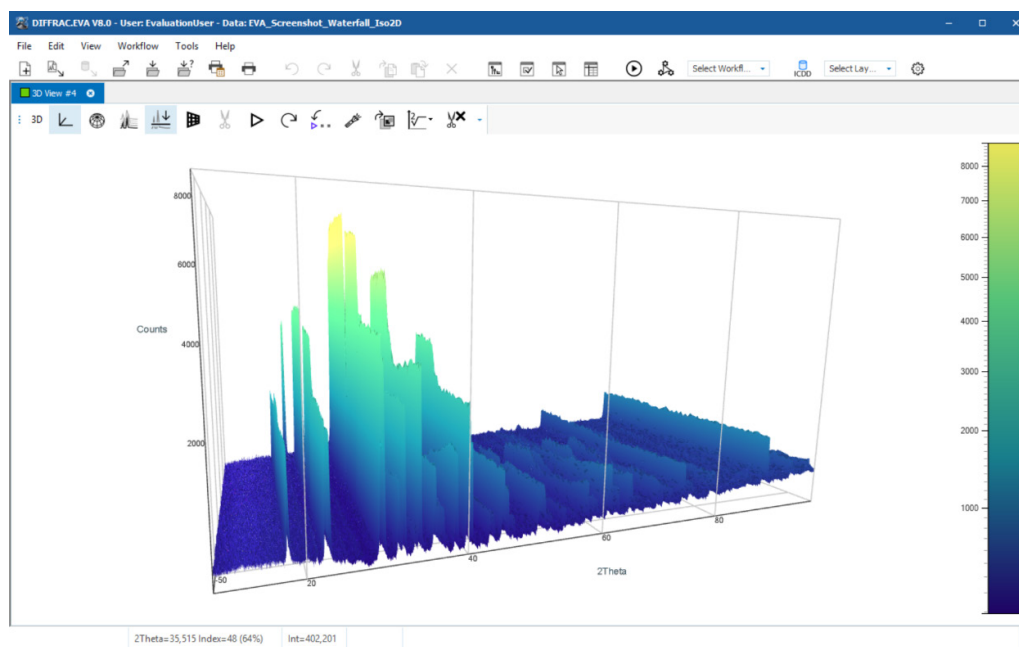


Figure 3

Evolution of powder XRD scans of NH_4NO_3 with temperature, shown as a hyper surface 3D view.

Workflow Automation and Productivity Enhancements

Workflow automation in EVA 8 has been significantly expanded:

- More commands are recordable in the **Workflow Editor**
- Workflow steps can be hidden to improve readability and simplify output at runtime.
- Workflows can be executed from the **command line**, optionally without showing the main window or with automatic closure after completion
- Batch execution across multiple scans or frames reduces repetitive manual work

The **Instant Runner** now displays step descriptions and closes automatically after execution, supporting a cleaner, more streamlined workflow experience. This enables unattended and reproducible analysis, supports high-throughput and QC environments, and reduces operator interaction and error risk.

In addition, EVA workflows now interact closer with the measurement software. Start Jobs and the Results Manager plugins can launch EVA workflows. The XRD ASSISTANT for reviewing scan data, automated BBE/EVA evaluation results as well as interactive EVA evaluation results stored in the database on desktop computers or tablets running web-based viewers (Windows, Apple, Android)

TOPAS Integration and BBE Automated Evaluations

EVA 8 supports **direct export of TOPAS pro-files**, aligned with DIFFRAC.TOPAS V8. In addition, EVA can directly launch TOPAS evaluations, preparing the ground for tighter integration with upcoming TOPAS versions. This creates a seamless transition from phase identification in EVA to advanced quantitative refinement beyond the EVA fit capabilities.

Released in parallel, **DIFFRAC.BBE 2.1** further strengthens automation of EVA by enabling:

- Automated Phase ID
- Creation of TOPAS quantitative refinement models
- Execution of EVA workflows
- PMI and SQUALL pattern matching

Together, EVA 8 and BBE 2.1 form a powerful automated evaluation pipeline.

Bruker AXS
info.baxs@bruker.com

bruker.com

Worldwide offices
bruker.com/baxs-offices



Online information
bruker.com/xrd-software

