



X-RAY DIFFRACTION DIFFRAC.EVA

Highlights, Capabilities & User Benefits

Summary

DIFFRAC.EVA is a versatile software package designed to streamline and enhance the analysis of one- and two-dimensional X-ray Diffraction (XRD) data. It integrates advanced algorithms, user-friendly design, and seamless connections with other Bruker software to deliver accurate and efficient phase identification, quantification, and microstructural analysis.

EVA employs data-driven algorithms aligned with AI and machine learning principles such as clustering, dimensionality reduction, pattern matching, and iterative refinement for enhanced phase identification and automation. It provides an intuitive, customizable GUI with real-time previews, advanced visualization options, and workflow automation for consistent, efficient handling of large datasets. DIFFRAC.EVA seamlessly integrates with Bruker's DIFFRAC.SUITE software, the instrument database and Results Manager, supporting regulatory compliance (cGxP/21 CFR Part 11).

DIFFRAC.EVA covers

- **Comprehensive Data Handling:** Supports 1D and 2D XRD data processing including scan arithmetics, smoothing, background determination, peak search, and conversion of 2D frames to 1D scans for detailed analysis, data presentation and reporting.
- **Advanced Analytical Tools:** Offers area analysis, peak profile fitting, rocking curve analysis, and corrections for sample displacement and spectral impurities treatment.
- **Phase Identification and Quantification:** Features a reliable industry-leading search/match module capable of simultaneous searches across multiple databases, combined XRD-XRF analysis for chemical consistency, automation, numerous traditional peak-stick and modern profile-fit residual search tools.
- **Whole Pattern Fitting:** Enables evaluation of crystalline and amorphous phase composition, lattice parameters, preferred orientation, crystallite size and microstrain.
- **Whole Pattern Matching:** Chemometrics and Similarity Analysis incorporates tools for High Throughput Screening, clustering, visualization of large datasets, quality control, detection of amorphous samples, semi-quantitative analysis (SQUALL) for crystalline and amorphous materials and Positive Materials Identification (PMI).
- **Pair Distribution Function (PDF) Analysis:** Generates experimental PDFs from raw data with automatic corrections, facilitating analysis of disordered or non-crystalline materials based on interatomic distances analysis and export for advanced cluster modeling in TOPAS.

Data-Driven by Design – Intelligence Where It Matters

DIFFRAC.EVA has long been recognized for its robust, data-driven algorithms—trusted by experts for their transparency, reproducibility, and scientific rigor. What’s increasingly clear is that many of these well-established techniques also align with the core principles of **modern artificial intelligence (AI)** and **machine learning (ML)**.

Users already rely on DIFFRAC.EVA’s tools for clustering, pattern matching, and automated analysis. These methods are grounded in well-understood mathematics and overlap with approaches commonly used in machine learning:

- **Cluster Analysis** groups patterns based on similarity without prior labeling—this is classic unsupervised learning, a foundational AI technique.
- **Dimensionality Reduction** tools like PCA and MMDS help interpret complex datasets—just as they do in AI for visualizing high-dimensional data.
- **Pattern Matching** uses correlation matrices and adaptive scoring—statistical similarity measures analogous to those used in classical pattern-recognition workflows.
- **Automated preprocessing** (e.g., background subtraction, amorphous detection) mirrors ML’s data preparation pipelines.

Unlike generic AI tools, DIFFRAC.EVA’s algorithms for phase identification are **interpretable and grounded in crystallographic logic**. They scale to thousands of patterns, integrate metadata, and adapt to real-world lab conditions—making them ideal for high-throughput environments in materials science, pharmaceuticals, and beyond.

- **Chemical filtering** and **database constraints** act as **domain-informed feature selection**, improving precision and reducing noise.
- **Residual Scans** and **Match Peak methods** apply **iterative refinement** and **selective processing steps**, directing analysis toward unexplained features—concepts central to modern ML models.
- **Optimization-based profile fitting** for residual phase detection reflects the same principles used in ML model training.

DIFFRAC.EVA bridges the gap between crystallographic tradition and intelligent automation. It empowers users to work faster, smarter, and with greater confidence—without sacrificing control or clarity. **A Modern Platform, purpose-built for Intelligent XRD.**

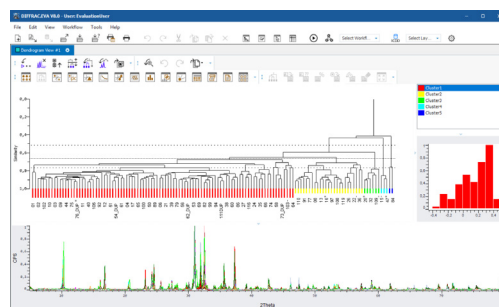


Figure 1 A combined view showing a dendrogram that groups the dataset by dissimilarity, the selection of a specific cluster, all associated scans, and a silhouette plot used to assess the compactness and separation quality of that cluster.

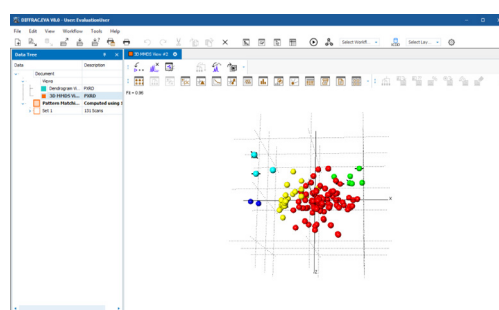


Figure 2 3D MMDS (Metric Multi Dimensional Scaling) visualizes the similarity relationships between scans—nearby points represent similar patterns, while groupings reveal clusters. A comparable separation can be achieved using 3D PCA (Principal Component Analysis). EVA offers both methods, which may provide different but complementary insights depending on the dataset.

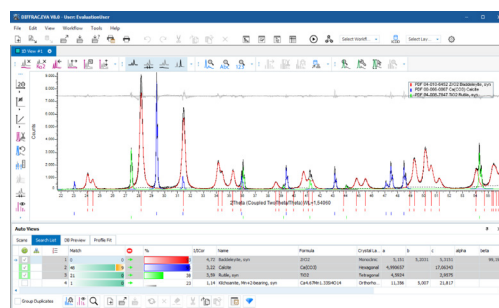


Figure 3 Profile Fit Residual Search (PFRS) combines optimization based profile fitting with chemical filtering, residual analysis, and heuristic rules to automatically detect minor and trace phases that remain hidden in complex or overlapping patterns.

Key Applications

DIFFRAC.EVA's core strength lies in its comprehensive toolkit for analyzing 1D and 2D XRD data. Its applications span across multiple domains:

Advanced Visualization – Insightful, Intuitive, Efficient

DIFFRAC.EVA is built around a user-centric design philosophy that emphasizes **intuitiveness, customization, and visual clarity**.

EVA offers a comprehensive suite of tools for advanced data analysis, visualization, and reporting—designed to support both routine workflows and cutting-edge research. It transforms complex XRD data into actionable insights with minimal effort.

Real-Time Feedback & Interactivity Powerful Visualization Tools

- The **Real-Time Preview** feature provides immediate visual validation of all evaluations. Advanced zooming, panning, and synchronized views and tables enhance data exploration in 1D views.
- Interactive elements like **context menus, mouse/keyboard shortcuts, and property panels** offer precise control over analysis and display.
- **Bragg 2D View:** A specialized view for **visualizing sample inhomogeneities** like spottiness, texture, or preferred orientation, particularly useful with Bragg-Brentano geometry and 1D detectors.
- **Multi-Scan Representations:** Customizable 2-D and 3-D multi-scan representations are available, such as iso-intensity and waterfall plots and true 3D surface plots. The waterfall display can include an additional "Side View" to visualize dependencies between scan properties (e.g., temperature, humidity, time, crystallinity or even charging states of batteries).

Reporting

- Supports a wide range of **visualization tools**, including Bragg2D, iso-intensity, and waterfall plots.
- Generates results **publication-ready figures** and **customizable reports** with integrated charts, tables, and annotations including picture-in-picture (PIP) and vertical-in-place (VIP) zooming.
- Includes a built-in **Report Writer** and extensive **data export options** for seamless integration with other tools like the Results Manager or generic spread sheet and office applications.

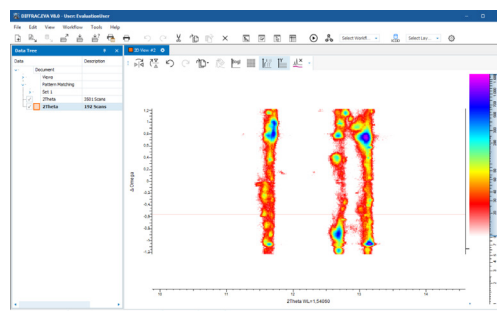


Figure 4 Bragg 2D provides a two dimensional visualization of diffraction signal inhomogeneities that reveal issues in sample preparation. This patented method enables rapid measurement and visualization of spatial crystallite distributions and size effects using only a standard 1D detector—no dedicated 2D hardware required (US16/044,940, EP19187229.0A, CN201910672756.3A)..

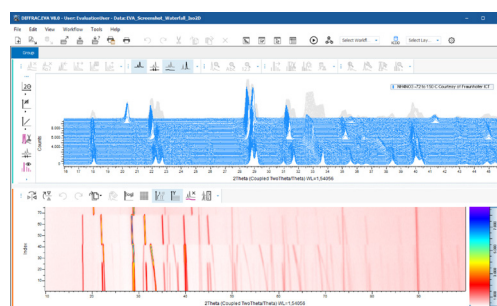


Figure 5 Overview of temperature dependent powder diffraction data shown as a waterfall plot and a 2D heat map. Both visualizations clearly reveal phase formation, lattice expansion, and symmetry changes—effects that are simply monitored through the shift and intensity evolution of the diffraction peaks.

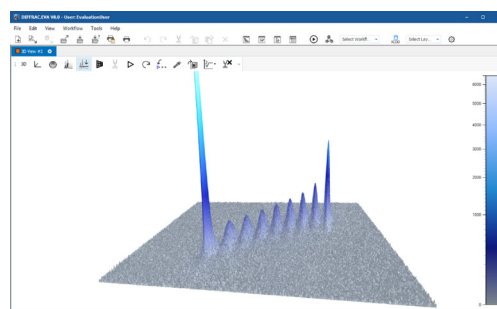


Figure 6 A reciprocal space map (RSM) derived from High-Resolution X-ray Diffraction Data (HRXRD). It visualizes the epitaxial relationship between the single crystal substrate and the deposited layers, revealing lattice matching, strain states, and the coherence of the crystalline stack in a 3D representation.

Reliable and Advanced Phase Analysis

DIFFRAC.EVA is a powerful software solution for phase identification and quantification, combining accuracy, flexibility, and ease of use. It leverages a **full-pattern approach** for highly reliable results, even with poor data quality or complex mixtures.

Core Capabilities

- **Phase Identification is inherently complex**, given the existence of nearly **one million known substances**. To improve efficiency and accuracy, all **DIFFRAC.EVA Phase ID algorithms** benefit significantly from **Search Space Reduction** tools. These include **chemical filters, database filters,** and customizable **phase white-lists and black-lists**, which help narrow down relevant candidates early in the process. By reducing irrelevant matches, these tools streamline the identification workflow and enhance the reliability of results. Additionally, **simultaneous searching across multiple databases** increases coverage and improves the likelihood of correctly identifying phases—especially in challenging or ambiguous cases. These strategies are universally beneficial across all EVA Search/Match algorithms.
- **Single Peaks Phase ID** (sometimes called 2nd generation phase identification) is a traditional, multi-step method for identifying crystalline phases from diffraction data. It begins with peak detection, where individual diffraction peaks are in the pattern. These peak positions can then be refined using peak fitting to improve accuracy. Next, the refined peak list is compared against phase databases to search for candidate phases. The user evaluates these candidates by checking how well their reference patterns match the observed peaks. The key tool in this process is the **Matching Lines View**, which provides a visual overview of which peaks are explained by which phases. It highlights assigned peaks, unassigned peaks, and missing data, making it easier to assess the quality of the match and refine the phase selection.
- **Full-Pattern Phase Identification** (or 3rd generation Phase ID) is the gold standard in phase ID. It utilizes all scan information—peaks, shoulders, and background—for robust identification. Simultaneous searches across multiple databases (ICDD PDF databases, COD, and user-defined) ensure comprehensive coverage. **Residual Search** identifies minor and trace phases through advanced residual analysis. **Automated Displacement Correction** corrects for sample height variations during search/match, improving reliability.
- **Combined XRD-XRF Analysis** integrates elemental data (e.g., from XRF) to restrict search/match to chemically consistent phases. This significantly improves identification success rates and enhances quantitative accuracy, specifically of substitutional mixed crystals.
- **Simultaneous Quantitative analysis** supports methods like **Reference Intensity Ratios (RIR)** and the **spiking method** for accurate quantification even of amorphous materials alongside identification.

Figure 7 A periodic table view with selected elements highlighted in blue, representing a predefined chemical filter—in this example, elements commonly occurring in rock forming minerals. DIFFRAC.EVA includes several such predefined filters, and users can adapt them freely by manual selection or by importing element lists from chemical analyses of the specimen.

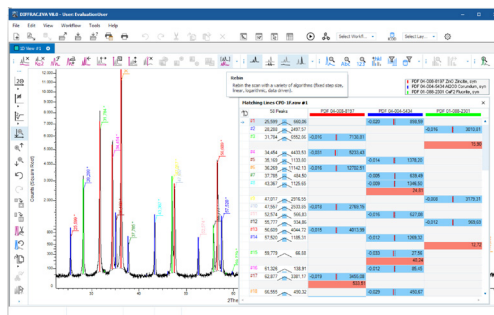


Figure 8 Illustration of traditional phase identification based on individual peak assignment. The inset shows the “Matching Lines View,” which aligns detected peaks in the scan with the expected reference signals from crystallographic databases. This workflow remains available for users who prefer manual control, while modern EVA versions also offer more automated, full pattern approaches for faster and more robust phase identification.

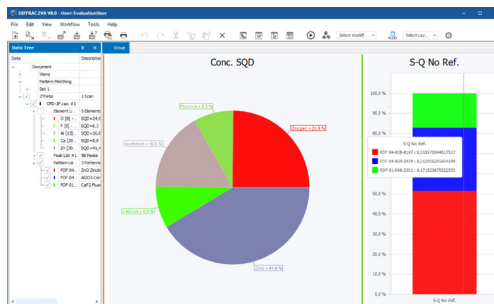


Figure 9 Results presentation based on the phase analysis from the previous figure. The stacked bar chart shows the relative phase concentrations, while the pie chart reflects the corresponding elemental composition derived from the identified phases and their stoichiometry. These charts are examples of EVA’s flexible reporting options, which also include tables, unstacked bar charts, line charts, and customized layouts that can be combined into comprehensive final reports.

Advanced Tools

- **PMI (Positive Materials Identification)** is the most basic form of material type assignment. Based on the SQUALL methodology, it offers rapid classification by correlating unknown samples with reference scans. Ideal for quick screening when the full phase breakdown isn't required.
- **SQUALL (Semi-QUantitative Analysis for aLL patterns)**
Introduced with version 6, SQUALL enables semi-quantitative analysis using full-profile PXRD data. It handles crystalline, amorphous, and unknown-structure materials, with minimal sensitivity to preferred orientation. All input it needs is reference scans that can be hosted in EVA's user database or can be loaded from the PDF5+ database. SQUALL weighted Ridge-Regression can provide automated phase identification (4th generation) or simply be used for quantitative analysis based on the RIR method
- **Improved Pattern Fitting**
Enhanced in V7, includes lattice parameter refinement, preferred orientation correction (March-Dollase or spherical harmonics), and amorphous content estimation. Supports Voigt and Pearson VII peak shapes for better microstructure analysis. **Profile Fit Residual Search (PFRS)** can interactively be used to find minor or trace phases in strongly overlapping multi-phase patterns.
- **DIFFRAC.TOPAS** structural and phase analysis is unprecedented in speed and stability. Combine EVA as advanced database search tool for phase identification and initial model building with the power of TOPAS's convolution based peak profile fitting and other advanced techniques. Simply create input files containing phase and crystal structure data in EVA and export them for deeper evaluation in TOPAS, or directly start the TOPAS refinement out of EVA.
- **EVA Core** EVA Core is the phase identification kernel of DIFFRAC.EVA used in automated workflows of DIFFRAC.BBE, our Black Box Evaluation software. Think of EVA Core as an **automated librarian for X-ray diffraction data**. Just as a librarian can quickly find specific books (phases) based on keywords (filters) within a vast collection of information (databases), EVA Core automatically identifies the crystalline phases present in your XRD data by searching through various crystallographic databases and applying specified heuristics, streamlining the process of characterization. This **is a key to closed-loop experiments** where an intelligent sample synthesis and preparation system integrated in an autonomous laboratory can create new materials based on the phase content determined in previous XRD experiments, while EVA may prove the novelty of the newly synthesized material.

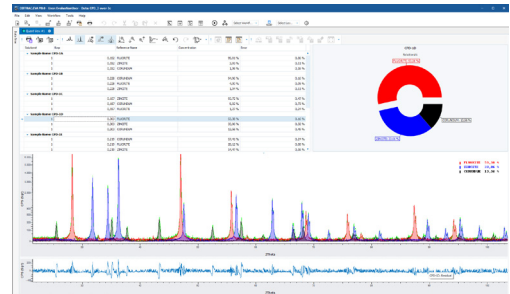


Figure 10 When no suitable database entries exist—or when profile fitting is not feasible due to the absence of an analytical peak profile model, as is the case for turbostratically disordered clays—DIFFRAC.EVA enables whole profile matching against a self collected library of representative reference scans. This approach supports 4th generation phase identification and quantitative analysis based solely on similarity between measured patterns and known reference materials.



Figure 11 An advanced environmental study demonstrating how automated phase identification with PFRS can be used to fingerprint the mineralogical composition of rooftop dust. The matching mineralogy clearly indicates its origin from Sahara Desert dust events, proving PFRS to be a valuable tool for identifying trace materials in complex environmental samples.

Pair Distribution Function (PDF) Analysis

Starting with license level 7, **DIFFRAC.EVA** enables the generation of experimental **Pair Distribution Functions (PDFs)** from raw diffraction data—an essential capability for analyzing disordered materials, nanostructures, or local structural effects. The process involves automatic corrections for background, Compton scattering, absorption, polarization, and X-ray fluorescence, followed by normalization and Fourier transformation using **PyTSRedX** algorithms.

PDF evaluation: Evaluating the structure databases for bond lengths and showing them as a Histogram overlay to the experimental PDF. Interactive PDF evaluation to identify bonds/coordination scenarios from PDF. Also, discrete interatomic distance pattern based on crystal structure data can be used for assigning PDF signals to local structures. The experimental PDF can then be exported for further quantitative evaluation of larger clusters in **DIFFRAC.TOPAS**.

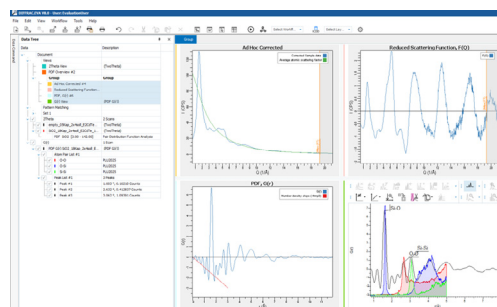


Figure 12 The upper left panel shows the diffraction pattern of amorphous or nano crystalline silica glass (SiO_2), followed by the intermediate processing steps and data correction. The resulting radial distribution function highlights interatomic distances, which are explained by the histogram shown on the right. The PDF reveals the characteristic tetrahedral short range order of silica, where each silicon atom is coordinated by four oxygen atoms in a tetrahedral arrangement. These tetrahedra are interconnected through shared oxygen atoms—similar to the local structural motifs found in crystalline silica (e.g., quartz).

Smart Chemometrics & Big Data Tools for High-Volume Analysis

DIFFRAC.EVA is built to handle the demands of modern high-throughput XRD workflows, offering powerful tools for managing, analyzing, and visualizing large datasets with speed and precision. Designed for **fast detectors and in-situ environments**, **DIFFRAC.EVA** streamlines high-throughput screening. The **Multi-Scan Reader** quickly loads and previews hundreds of scans, allowing users to extract and focus on patterns of interest with ease

The integrated Cluster Analysis module—based on the proven POLYSNAP software—groups and visualizes thousands of diffraction patterns by similarity. This enables rapid identification of trends, outliers, and phase similarities, making it ideal for polymorph screening, salt selection, and exploratory data analysis. It drives efficiency in analyzing large amount of data and samples by grouping those for similarity, creating interactive TOPAS refinement models per cluster using the most representative cluster members and batch refining all cluster members using the **DIFFRAC.BBE** tool for automated data evaluation.

A dedicated **Quality Control mode** compares new measurements against reference patterns to detect deviations. It highlights unstable or non-conforming samples, supporting long-term material monitoring and pass/fail decisions.

EVA's advanced views used in cluster analysis comprise:

- **Cluster Analysis Views:** Offers a rich set of graphical tools including **Cell Display**, Well Plate View, **Dendrogram**, **3D MMDS**, **3D PCA**, **6D Plot**, and validation views like **Scree Plot**, **Silhouettes**, and **Parallel Coordinates**.
- **6D Plot:** Visualizes additional sample preparation information (e.g., mass, solvent, temperature) in up to three extra dimensions (point size, shape, color), helping to discover connections between preparation conditions and resulting clusters.

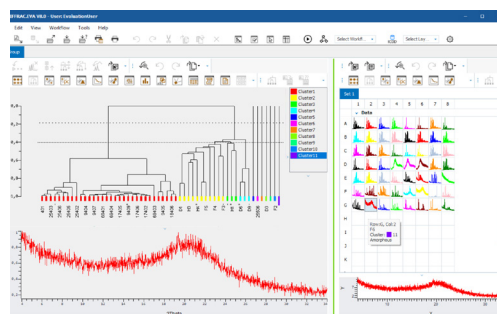


Figure 13 High throughput screening of pharmaceutical samples prepared in a well plate. The dendrogram highlights several outliers, which can be directly traced back to their respective wells in the panel on the right. The selected outlier is identified as amorphous, demonstrating how EVA rapidly distinguishes amorphous from crystalline samples in large screening campaigns.

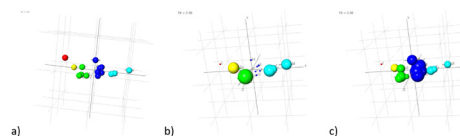


Figure 14 The 6D plot visualizes up to six dimensions of information simultaneously. The spatial distance between spheres represents the similarity of cluster members, while color distinguishes the individual clusters. Additional dimensions can incorporate metadata—here, sphere size reflects elemental enrichment in iron ore samples from Brazil. Panel (a) shows the 3D MMDS view of the dataset, and the 6D representation further highlights low Ca concentrations (b) and high Ti concentrations (c) within the blue cluster.

Technical Overview – Built for Performance and Compatibility

DIFFRAC.EVA is engineered to take full advantage of modern computing environments, ensuring smooth operation, high-speed processing, and seamless integration within the Bruker software ecosystem.

Intuitive & Customizable Interface

- A **clean, modern GUI** with large, color-coded icons and grouped toolbars simplifies navigation and reduces the number of steps for common tasks.
- Users can fully **customize layouts, toolbars, and screen settings**, which are saved with project files for seamless continuity.
- The **data tree** allows flexible organization, sorting, and visibility control of scans, patterns, and results.

System Requirements & Compatibility

- **Operating Systems:** Fully compatible with **Windows 10 and 11**.
- **64-bit Architecture:** Required from **version 7.0** onward for installation and operation.

Performance Optimization

- **Multi-Core Processing:** Key features like **Cluster Analysis, Search/Match**, and **Database Compilation** are multithreaded for faster execution.
- **Graphics: Hardware-Acceleration** for 2D and 3D views provide smooth interactivity for large amounts of data, and **vector-based icons** allow for crisp display on high-resolution screens.

Database Support & Management

- **Supported Databases:** Includes ICDD PDF2, PPDF5+, PDF 4 AXIOM, Minerals and **COD (Crystallographic Open Database)**. User-defined databases are also supported.
- **Database Tools:** Offers utilities for **compilation, updates, filtering, and data mining**, with multithreaded DSRD compiler for efficient processing.
- **Access & Licensing:** Supports **server-based licenses** and **web-based databases** (e.g., PDF-4+ Web), with internet access required for license validation.

Support

- **Free Maintenance Updates:** Ensure access to the latest bug fixes and improvements.

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