



## X-RAY DIFFRACTION

# DIFFRAC.XRD ASSISTANT

## Simplifying XRD for Everyone

**XRD ASSISTANT** is a modern web application designed to make X-ray diffraction (XRD) measurements, evaluations, and instrument management more accessible than ever. With its intuitive interface, real-time monitoring, and immediate result presentation, it's especially well-suited for occasional users and non-experts who need reliable insights without navigating complex software environments.

Whether accessed as a standalone browser-based app—on desktop or mobile—or integrated as a plugin within the **DIFFRAC.MEASUREMENT** framework, XRD ASSISTANT offers a streamlined experience tailored to both casual users and seasoned professionals.

At its core, the software provides a simplified interface for operating XRD instruments, monitoring hardware status, launching measurement jobs, and reviewing results. Users can easily assign templates to specimens using a graphical loader, track job progress in real time, and view evaluation results immediately after completion. The **Analysis Library** connects directly to the instrument's result database, allowing users to filter, query, and visualize scan data, phase identifications, fit curves, and more—all through interactive tables and charts. For quality control, XRD ASSISTANT supports statistical evaluations across multiple measurements, with progress charts, warning indicators, and out-of-range highlighting. Users can also generate professional PDF reports with just a few clicks.

The software is designed with usability in mind. Its responsive layout adapts to different screen sizes, making it ideal for desktop use but also permits tablet use and touch-screen operation. Multi-language support (English, French, Japanese and German), optional help fly-outs, and a clean, modern design ensure a smooth onboarding experience. Templates can be marked as favorites for quick access, and the interface is intentionally reduced to essential information—delivering power without complexity.

From a data security perspective, XRD ASSISTANT interfaces with the instrument's user administration system, ensuring data integrity and consistency. Users operate in a controlled environment where evaluations are displayed but not modified, maintaining alignment with the main software.

## Home – Your First Point of Contact with XRD ASSISTANT

Upon launching the **XRD ASSISTANT** app, users are greeted by the **Landing Page**, also referred to as the **Home Screen** in the navigation. This is the central **hub** for interacting with the instrument—designed to provide a quick, informative overview and fast access to key functions.

At a glance, users can immediately assess the **Instrument Status**: is the system ready to measure? If not, shortcut buttons are available to initialize drives or start the generator—depending on system permissions. And when deeper diagnostics are needed, a direct link leads to the full Instrument Status page with a single click.

The **Start Jobs** section displays groups of template tiles, offering a fast way to launch measurement workflows. A refresh option ensures the latest templates are always visible, and users can jump directly to the full Start Jobs page for more control.

The **Analysis Library** area highlights recently completed jobs in a compact table view. Each entry includes a direct link to its detailed evaluation, making it easy to follow up on results or continue analysis. A general shortcut to the full library is also available.

The **Job Monitor** provides real-time visibility into the measurement queue, showing running and pending jobs. Users can access the full job monitor page directly from this section to manage or review job progress.

### Toolbar elements

At the top of the screen, a **toolbar common to all pages** provides access to essential controls: a menu dropdown, links to connected instruments, and a service menu for changing language, logging out, or toggling browser into full-screen mode.

A **notification area** keeps users informed of the latest system messages, while the **Help** command toggles an overlay of contextual help fly-outs—making it easy to get assistance without leaving the page.

Designed for clarity and speed, the Home Screen ensures users can move from overview to action in seconds—whether they're starting a job, checking system readiness, or diving into analysis.



**Figure 1**

Tablet View of the XRD ASSISTANT Home screen, a Responsive user interface optimized for touch operation.

## Start Jobs – Launching Measurement and Evaluation Workflows with Ease

Starting a measurement or evaluation job is made intuitive and efficient using **templates**—predefined workflows imported directly from the instrument database. These templates, or template groups, can be displayed either as **tiles** for quick visual selection or in a **tabular format** for more detailed inspection.

During import, each template is automatically verified against the current instrument configuration. In the tiles view, only matching templates are shown, ensuring users only see what's ready to run. In the table view, all templates are listed, with matching ones clearly flagged as "OK." This view also provides additional metadata about each template, helping users make informed decisions. Templates can be marked as **favorites**, making them easily accessible via the dropdown menu—ideal for frequently used workflows. For example, a verification template marked as a favorite appears with a small asterisk in the upper right corner of its tile.

Launching a job follows a straightforward workflow: users can either click the tile or select a template from the table and press the **Start Template** button in the page toolbar. The workflow begins with a setup step, prompting the user to enter the **specimen name**. If a sample changer is configured and the template doesn't specify fixed sample positions, the user selects positions interactively from a graphical loader view. Multiple samples can be selected to run the same template, with specimen names assigned individually.

Naming specimens is flexible and can be done manually or dynamically by combining text with variables such as serial number, instrument name, user ID, user name, sample position, template name, and more. This ensures consistent naming conventions and traceability across jobs, while also saving time in repetitive workflows.

Once a measurement has been started, XRD ASSISTANT automatically switches to a Live View, providing immediate visual feedback on the ongoing scan. As the measurement progresses, users can observe how the diffraction pattern evolves in real time. This live monitoring capability increases transparency and confidence during routine operation, allowing users to verify correct execution early and react promptly if unexpected behavior is observed.

After the scan is completed, and if an evaluation is defined in the selected template, the evaluation is executed automatically—typically by invoking DIFFRAC.BBE and its associated evaluation workers. The live scan display seamlessly transitions into an evaluated scan view, showing stick patterns for phase identification or fitted curves from profile analysis performed with TOPAS or EVA. Numerical evaluation results are presented in collapsible tables and charts, adapted to the analysis type—for example, pie or bar charts illustrating phase concentrations in semi-quantitative or Rietveld-based quantitative analyses. This immediate transition from measurement to evaluated results ensures a smooth, end-to-end workflow from data acquisition to actionable insight.

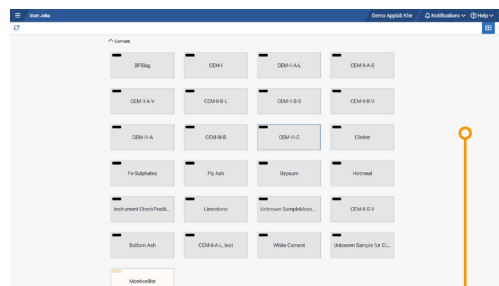


Figure 2  
Template selection

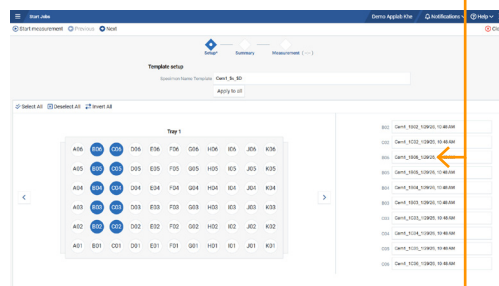


Figure 3  
Sample assignment



Figure 4  
Scan Live View

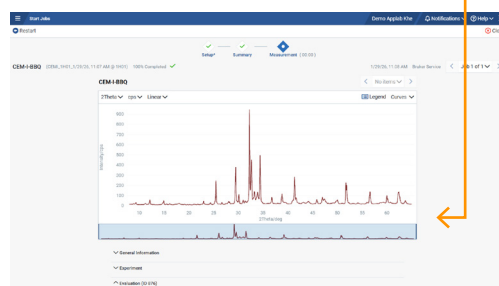


Figure 5  
Evaluation and results presentation. One continuous workflow from data acquisition to evaluated results.

## Analysis Library – Seamless Access to Instrument Data and Evaluation Results

The **Analysis Library** is your gateway to streamlined data access and powerful insights. It connects directly to the instrument database, enabling users to **view measurement data**—including various defined types—and their **associated evaluation results** with ease.

### Single-Sample Data – Deep Dive into Individual Evaluations

The Single-Sample Data functionality focuses on evaluations performed on individual samples, offering a structured yet flexible way to explore results. Each analysis type—whether it's phase identification, quantitative or semi-quantitative analysis, peak and area evaluation, or residual stress measurement—is represented in a standardized format, ensuring consistency and comparability across datasets.

Beyond these predefined types, the system also supports more generic evaluation results. These can be injected into the database as key-value pairs, allowing for flexible data capture even when no dedicated representation is available. While such entries appear as simple lists, users can still refine their view by applying additional filters, narrowing down results based on scan-specific metadata. These queries are tied to individual scan evaluations and are presented in an overview pane, which can be expanded into a detailed view for deeper inspection.

Although the term single sample refers to the evaluation of one scan at a time, multiple scans and evaluations often belong to a broader measurement or evaluation job. The detailed view allows users to browse through these related scans, providing a comprehensive picture of the entire job.

The detailed view furthermore shows a graphical representation of the scan, including measured data, fit and difference curves, peak markers, and stick patterns for phase identification. The interface is interactive, allowing users to zoom, pan, adjust axis scales, toggle data items and legends, and explore the scan in a way that suits their workflow.



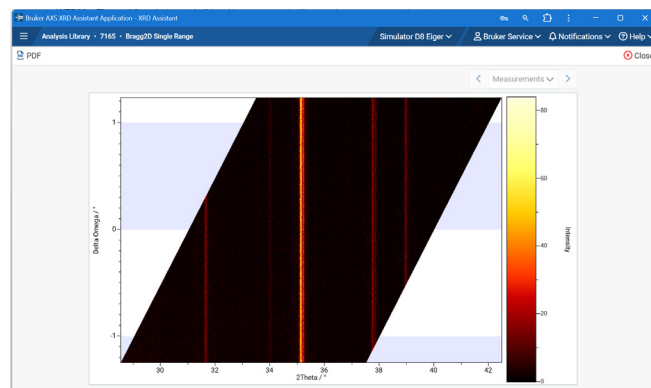
**Figure 6**

**Phase Identification – 1D Scan View:** 1D diffraction scan with phase identification results. Measured data are displayed together with stick patterns for identified phases. Interactive phase “pills” allow individual phases to be toggled on or off for focused visual inspection.



**Figure 7**

**Profile Analysis – Standardized Fit View:** Standardized profile-fit visualization for powder diffraction data. Measured intensities, fitted curves, difference plot, and peak markers are shown in a unified view, independent of whether the analysis originates from EVA pattern fitting or TOPAS Rietveld-style profile refinement.



**Figure 8**

**Bragg2D View – Sample Homogeneity at a Glance:** Bragg2D representation for rapid assessment of sample homogeneity. This two-dimensional view provides an intuitive visualization of crystallite size and distribution effects, offering fast insight into sample uniformity and potential inhomogeneities.

All numeric data and meta information provided by the evaluation software is displayed in customizable tables. For standardized data types—such as areas, peaks, patterns, or stress evaluations—users can tailor the table layout to highlight the information most relevant to them. Phase-specific properties like lattice parameters, symmetry, microstructure data, quantification values, and database references are grouped into expandable sections called harmonicas, keeping the interface clean while offering rich detail on demand. The wt-% concentration serves as the master property for each phase, anchoring the quantitative interpretation.

To support visual analysis, the system also offers pie as well as horizontal or vertical bar charts that illustrate specimen composition at a glance. For area and peak data, users can review microstructure details, position and intensity values, and shape characteristics, all within a unified interface.

Stress evaluations go a step further, combining graphical peak representations with detailed numeric tables. Users can view scalar stress states or dive into full tensor representations, depending on the depth of analysis required. This comprehensive approach ensures that specialists can extract precise insights from every scan, while also enabling clear communication of results across teams.

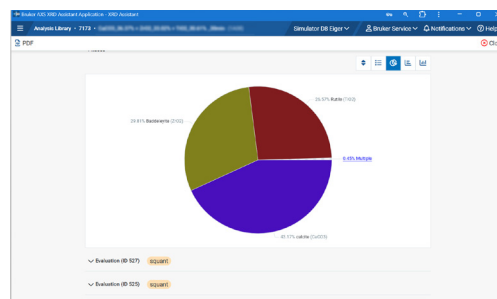
### Multi-Sample Selections – Broader Context, Smarter Insights

Beyond individual scan evaluations, the software offers a powerful way to analyze data across multiple samples using predefined views. These views are created in the **RESULTS MANAGER** and read directly from the instrument database. By selecting a view, users instantly filter the dataset to show only entries that match the view’s definition—ensuring that the data presented is both relevant and formatted according to the intended analysis context.

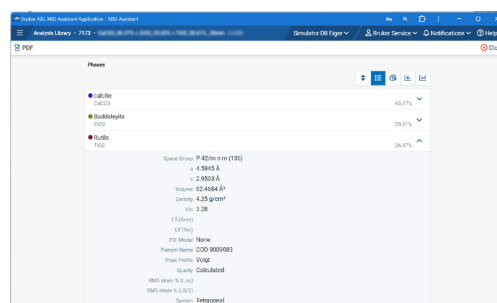
Once a view is selected, users can define a range of scans to include in the analysis. For this selection, the system generates **statistical summaries** of the results, which can be visualized either as **time series** or as **comparative charts** across different samples. This functionality is particularly valuable for identifying trends, spotting anomalies, or validating consistency across production batches or experimental runs.

In addition to the core data, the visualizations and tables also highlight **warnings** and **alarm conditions**, such as minimum or maximum value violations. These alerts help users quickly identify outliers or potential issues, supporting faster decision-making and quality assurance.

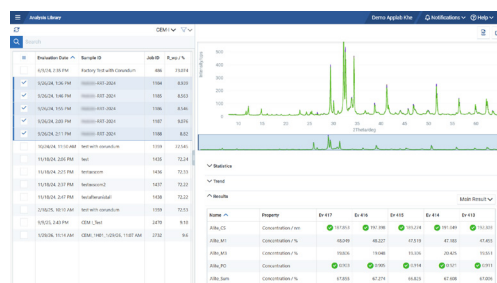
By combining structured views with flexible scan selection and rich visualization, the multi-scan functionality turns raw data into actionable insights—ideal for both routine monitoring and in-depth analysis.



**Figure 9**  
Quantitative Analysis – Concentration Overview: Phase concentration results visualized as pie or bar charts. Quantitative analysis results are displayed clearly, with minor phases below a configurable threshold automatically grouped as Multiple for improved readability.



**Figure 10**  
Numeric Results – Meta Information: Configurable tables for numeric results and phase metadata. Evaluation results and associated phase information are presented in tables, allowing users to focus on the most relevant numeric values and properties.



**Figure 11**  
Trend Analysis – Monitoring Results Over Time: Trend charts for quality monitoring and process control. Time-based charts visualize the evolution of measured and evaluated properties, including warning and alarm limits as well as optional moving or floating averages.

# Applications · Users · Benefits — One XRD Workflow for Every Laboratory

## Applications

XRD ASSISTANT supports a broad spectrum of routine and advanced XRD applications, enabling laboratories to standardize workflows without sacrificing analytical depth. Typical applications include automated quantitative phase analysis using TOPAS, TOPAS BBQ, or DQUANT; semi-quantitative analysis with EVA (RIR, full-pattern fit, PMI, SQUALL); interactive and automated phase identification with EVA and EVA Core; crystallinity analysis and peak monitoring based on peak fits or area evaluations; as well as materials research using LEPTOS X, and other DIFFRAC.BBE-based workflows.

## Users

XRD ASSISTANT is designed to serve all user roles within a laboratory through a single, consistent interface. Operators benefit from a simplified, fault-tolerant environment for executing predefined measurement and evaluation templates. Experienced users and lab managers define methods, templates, and result views in the main DIFFRAC software, which can then be executed reliably by laboratory staff. Supervisors and quality managers gain remote access to results, trends, and instrument status—supporting oversight and decision-making without requiring physical presence at the instrument.

## Benefits

The result is a unified, workflow-driven XRD experience that transforms complex diffraction tasks into repeatable, transparent, and accessible processes. By separating expert method definition from routine execution, XRD ASSISTANT increases efficiency, improves consistency, and lowers the barrier to high-quality XRD analysis.

Whether used in industrial quality control environments, where robustness, reproducibility, and fast decisions are critical, or in research- and R&D-focused academic laboratories, where insight, flexibility, and data transparency matter most, XRD ASSISTANT reflects how X-ray diffraction is operated today—connected, automated, and accessible to every user level.

## System Requirements

- Minimum resolution: 1024×768 px
- Supported browsers: Windows Chromium-based (e.g., MS Edge, Firefox, Chrome), Android from v10, iPadOS and Safari from 18.2
- Desktop integration: Windows 11 LTSC, 64-bit
- Instrument software versions: 8.8
- Supported scan types: 1D scans, range scans, step or continuous scanning, fixed detector, Bragg 2D, Variable Counting Time (VCT), Variable Step Size (VSS), Fix and variable Divergence Slit, Dynamic Beam Opening (DBO)

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