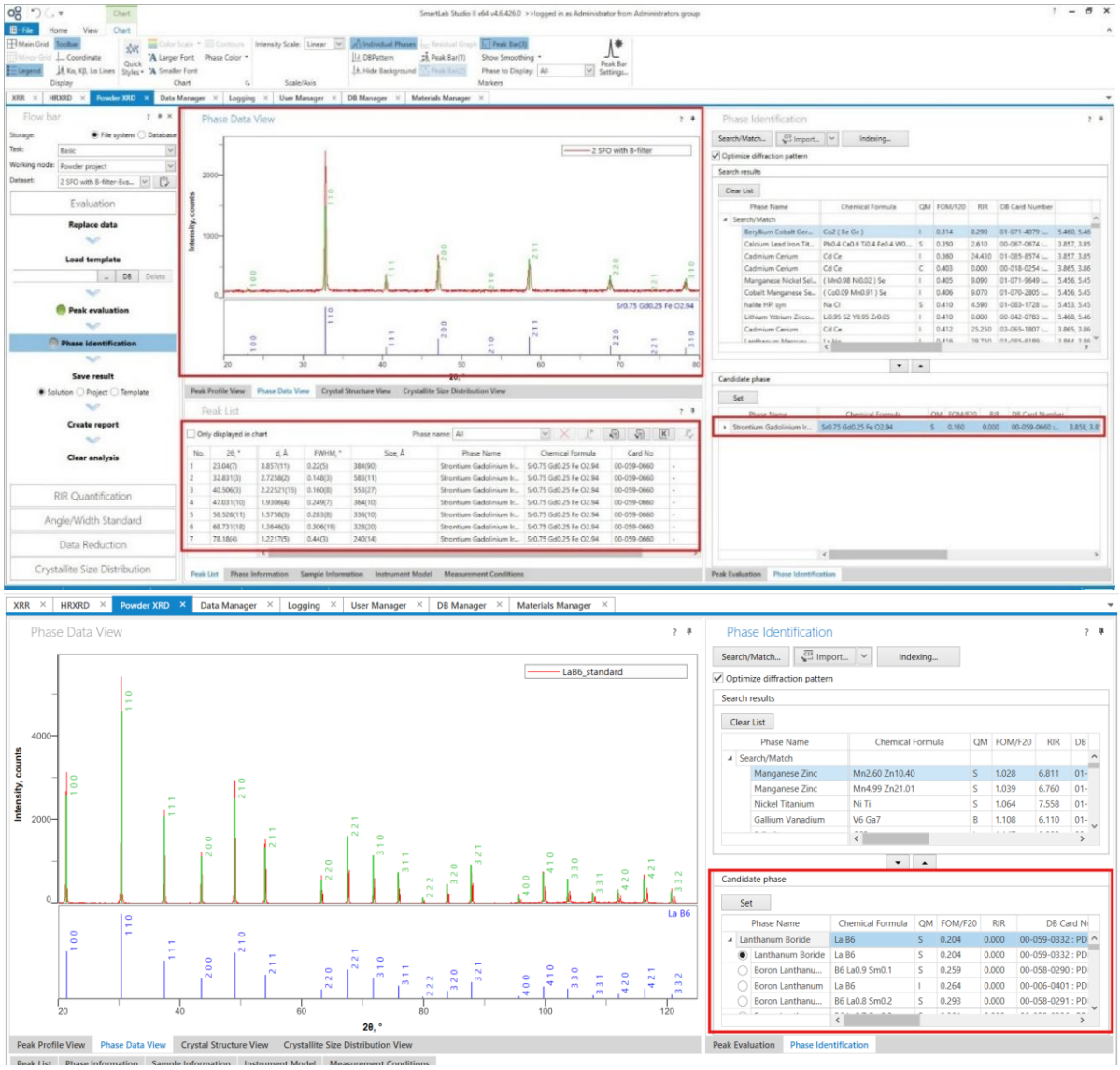
XRD Operational Manual Part-I: Qualitative Phase Identification Analysis Using SmartLab Studio II

Version: Basic-02-03-26

Other XRD Operational Manuals



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XRD Operational Manual Part-I: Qualitative Phase Identification Analysis Using SmartLab Studio II

Contents

Basics of XRD Analysis

XRD Operational Manuals

Basic (qualitative) XRD analysis relies on correctly linking measured diffraction peaks to the underlying crystal structure. A working understanding of crystal systems and Bravais lattices, symmetry operations (point groups and space groups with systematic absences), and Miller indices (hkl) is essential. These fundamentals support reliable peak assignment and accurate phase identification, forming the scientific basis of the Basic analysis workflow.

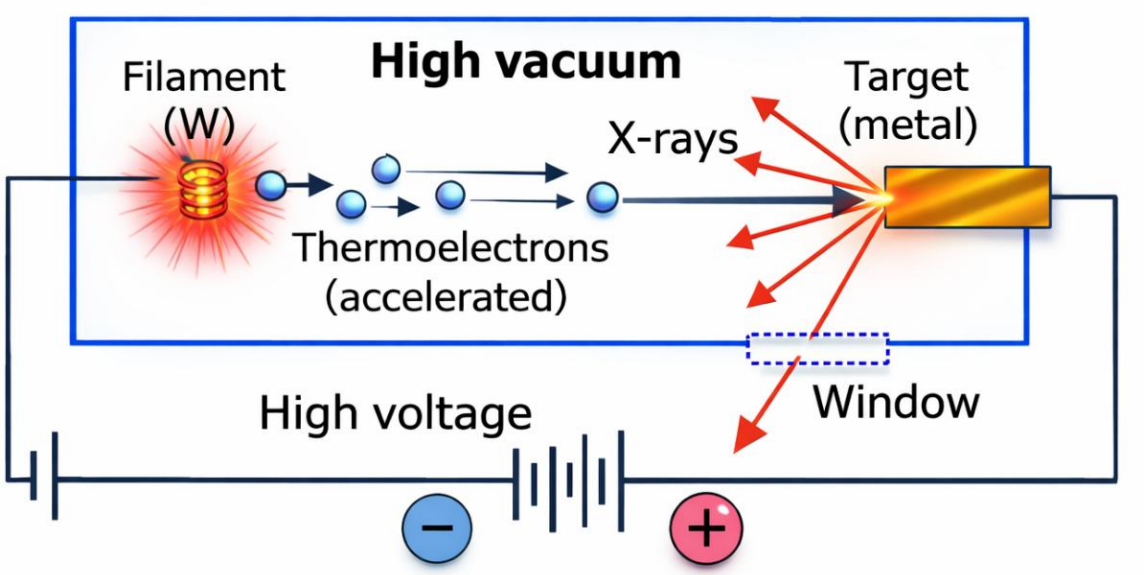
Measurement Data

Link

Measurement data are the foundation of both qualitative phase identification and quantitative XRD analysis, and their quality directly determines the reliability of any evaluation in SmartLab Studio II. Data quality is inherently purpose dependent: a scan optimized to detect weak phases prioritizes intensity and counting statistics, whereas a scan intended to separate closely spaced reflections or refine lattice parameters prioritizes angular resolution and peak-position accuracy. In the SmartLab SE, this optimization is achieved by choosing the appropriate optical configuration and scan conditions such as divergence and receiving slit settings, Kβ filtering or monochromation, step size, counting time, and 2θ range while maintaining correct alignment and a low, stable background to maximize signal-to-noise. When these parameters are matched to the analytical goal, the dataset contains sharp, correctly positioned peaks with reliable intensities, enabling robust identification and quantification; therefore, a tailored, optimized scan is far more valuable than a generic “typical” scan, and it is the researcher’s responsibility to ensure the data are clean, complete, and reproducible before import into SmartLab Studio II.

Generation of X-Rays

X-rays are generated in an X-ray tube when a heated filament emits electrons (thermionic emission) and a high voltage accelerates them toward a metal target (anode). When these fast electrons strike the target, their kinetic energy is converted into X-rays (and heat). Bremsstrahlung (braking) X-rays are produced when electrons are rapidly decelerated or deflected by the electric field of target nuclei, creating a continuous spectrum of X-ray energies. Characteristic X-rays are produced when an incoming electron ejects an inner-shell electron of the target atom, leaving a vacancy. An outer-shell electron then drops into the vacancy and emits an X-ray photon with a discrete energy specific to the target material.

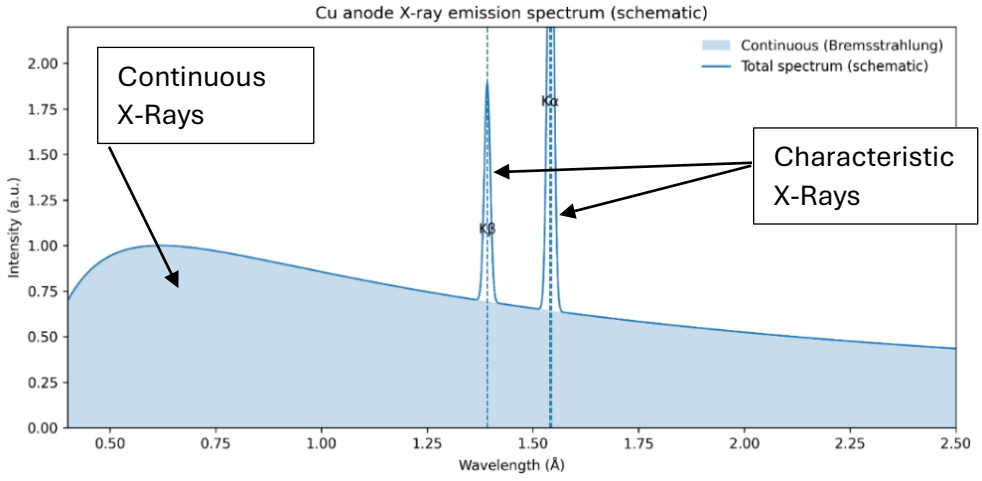


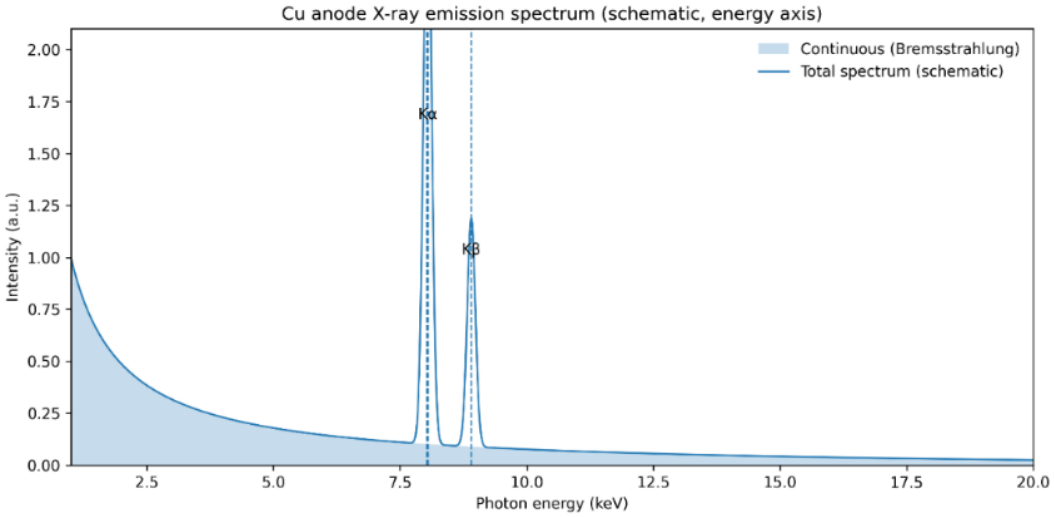
Cu is the general-purpose choice for most powders because it gives strong intensity and a wavelength suitable for many common lattice spacings. Longer wavelength (Cr or Co) are preferred when Cu causes strong fluorescence in Fe/Co/Ni-rich samples, since they lower background and improve peak visibility. Shorter wavelength (Mo or Ag) are used when greater penetration is needed for highly absorbing/heavy or thick samples, and when reflections from very small d-spacings must be measured within the instrument's available 2θ range. For very small d-spacing, Bragg's law requires a shorter wavelength to satisfy the diffraction condition. Thus, smaller-wavelength targets are used to keep diffraction angles measurable and avoid overlap at very high 2θ. Fe targets are less common in routine work but can be chosen for specific material constraints or lab standards where an intermediate wavelength gives cleaner data. Because of Bragg's law ($2d \sin\theta = \lambda$): smaller d-spacing requires larger θ, so those planes diffract at higher angles than planes with larger d-spacing.

Target Element	Atomic number	K-ray excitation voltage (kV)	Kβ (Å)	Kα1 (Å)	Kα2 (Å)	Kα (Å)
Cr	24	6	2.08491	2.28975	2.29365	2.29105
Fe	26	7.1	1.75665	1.93608	1.94002	1.93739
Co	27	7.7	1.62075	1.789	1.79289	1.79029
Cu	29	8.9	1.39225	1.54059	1.54441	1.54186
Mo	42	20	0.6323	0.70932	0.71361	0.71074
Ag	47	25.5	0.49729	0.55942	0.56381	0.56089

Kα and Kβ lines

Characteristic X-rays from a Cu anode are dominated by the Kα and Kβ lines, produced when an outer electron fills a vacancy in the K-shell: Kα comes from an L → K transition, while Kβ comes from an M → K transition, so Kβ has higher energy (shorter wavelength) than Kα. Importantly, "Cu Kα" is actually a close doublet $K\alpha_1$ (≈1.540562 Å) and $K\alpha_2$ (≈1.544390 Å) caused by subshell (spin–orbit) splitting, and it can produce slight peak doubling unless $K\alpha_2$ is suppressed/stripped (e.g., with monochromation). In powder XRD, any remaining Kβ component can satisfy Bragg's law at different angles and may create extra weak or shifted reflections, complicating peak assignment, therefore, Kβ is typically reduced by filtering or monochromation so the pattern is measured with (nearly) a single Cu Kα wavelength for more reliable interpretation. For Cu radiation, the intensity ratio of $K\alpha_1$ to $K\alpha_2$ is approximately 2:1, and the combined Kα intensity is about 6–7 times stronger than the Kβ intensity. By Bragg's law, shorter wavelength → lower 2θ, so Kβ (and $K\alpha_1$) appear left of Kα.



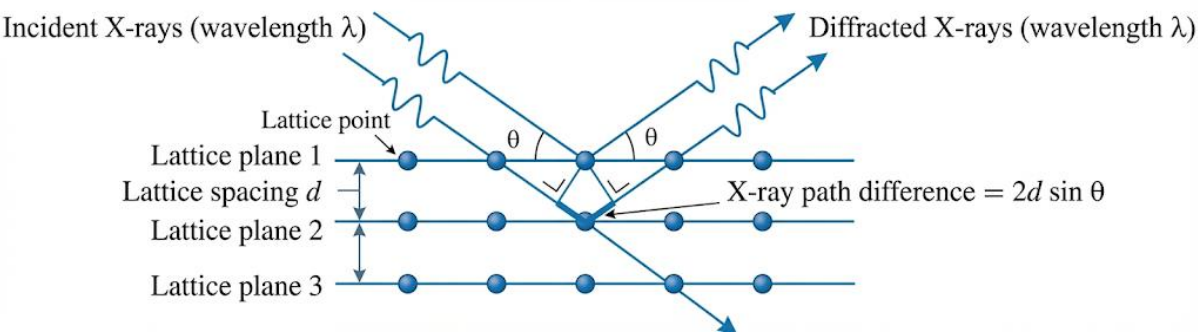


Powder XRD Method

Laue discovered that the scattering of x-rays (waves) is the process of diffraction from a crystal (like grating). Bragg discovered that this diffraction is from a set of parallel planes, so the diffracted beam appears to be specularly reflected from Crystal lattice planes. Thus solved the mystery of crystal structure. In the powder X-ray diffraction (XRD) method, a crystalline powder contains many tiny grains oriented randomly, so many sets of lattice planes are able to satisfy the Bragg condition during the scan. Constructive interference (diffraction) occurs when the optical path difference between X-rays scattered by parallel lattice planes with spacing $d$is an integer multiple of the X-ray wavelength λ. This is expressed by Bragg's law:

$$2d\sin\,\theta = n\lambda$$

Peaks appear at angles where this condition is met, allowing determination of interplanar spacings d and phase identification.



X-Ray Diffraction Patterns

1) Diffraction pattern

A powder XRD pattern is a fingerprint of the crystalline phases present in a sample. The set of peak positions (and their overall distribution across 2θ) reflects the allowed lattice-plane spacings, while the background shape carries information about non-crystalline contributions and instrument/sample scattering. Sharp, well-defined peaks typically indicate a crystalline material, whereas a broad diffuse hump is characteristic of amorphous or poorly ordered structure. By comparing the observed peak set to reference patterns, the pattern quickly reveals whether the sample is single-phase, multi-phase, or contains an amorphous fraction.

2) Diffraction peak width

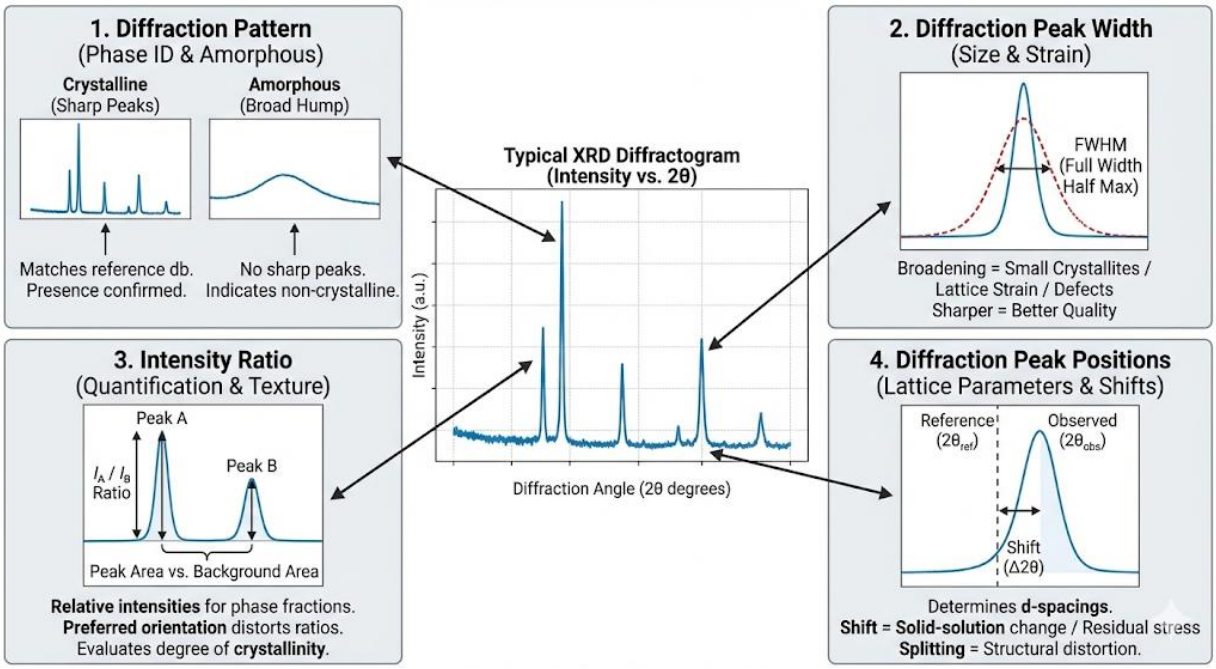
Peak width (commonly reported as FWHM) provides insight into the microstructural quality of the material. Peaks broaden when the coherent scattering domains are small (small crystallite size) and when the lattice contains distributions of spacing caused by microstrain, dislocations, and defects. Narrow peaks generally indicate larger crystallites and better long-range order, while broad peaks suggest nanocrystallinity or significant strain. With appropriate corrections for instrumental broadening, peak-width methods (e.g., Scherrer and strain-based models) can be used to estimate crystallite size and microstrain trends.

3) Diffraction intensity ratio

Diffraction intensity ratio means comparing the relative heights/areas of different peaks in an XRD pattern. These ratios can help estimate how much of each phase is present in a mixture, but they can also change if the sample has preferred orientation (texture) or other effects (e.g., absorption or particle statistics), so the ratios may not match the database perfectly. A strong peak-to-background contrast generally indicates higher crystallinity, while weak peaks on a high background suggest lower crystallinity or more amorphous content.

4) Diffraction peak positions

Peak positions (2θ) are the most fundamental measurable in XRD because they directly determine d-spacings through Bragg's law, and therefore the lattice parameters of the crystal. Reliable peak positions enable phase identification, indexing, and detection of structural changes. Systematic shifts of peaks to higher or lower 2θ can indicate lattice contraction/expansion due to solid-solution composition, temperature effects, or residual elastic strain. Peak splitting or additional shoulders often signals symmetry changes, phase coexistence, stress states, or distortions, making peak positions a primary indicator of structural evolution.



Crystal systems and the Bravais lattices

Crystal systems classify crystals based on the shape of the unit cell, defined by the edge lengths $a, b, c$and the angles α, β, γ. According to these relationships, crystals are grouped into seven crystal systems. Bravais Lattice describes the distinct 3-D arrangements of lattice points formed by combining each crystal system with possible lattice centerings (P, I, F, C, or R). This results in 14 unique lattices that represent all possible periodic crystal structures.

Qualitative Analysis in XRD

Qualitative XRD analysis in SmartLab Studio II identifies the crystalline phases present by importing the measured scan, verifying 2θ coverage and background, detecting and refining peak positions and relative intensities, and then performing a search–match against crystallographic databases. The output is a list of candidate phases whose reference patterns best reproduce the observed peaks and key intensity relationships, confirming which phases are present. This workflow implemented with tools such as peak evaluation and database matching does not determine how much of each phase is present; a separate quantitative method is required for that.

PDF-2

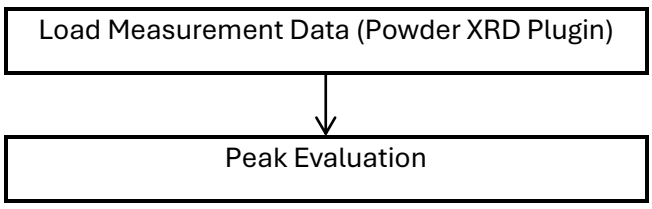
https://www.icdd.com/pdf-2/

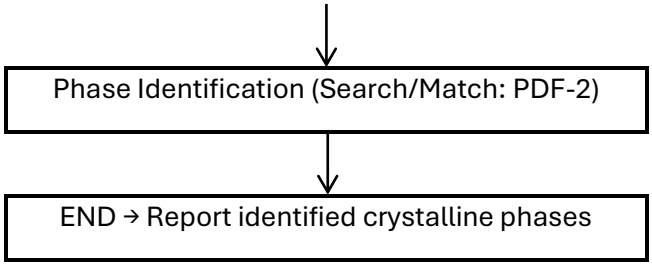
With the PDF-2 database integrated into SmartLab Studio II, one can perform standard qualitative phase identification of crystalline materials using powder XRD data. PDF-2 provides d-spacings, relative intensities, chemical formulas, crystal systems, and basic crystallographic metadata, enabling reliable Search/Match operations against measured diffraction patterns. Practically, this allows rapid identification of unknown phases, confirmation of expected phases in synthesized materials, detection of secondary or impurity phases, and routine phase screening in polycrystalline samples. PDF-2 is therefore well-suited for first-level material characterization, where the objective is to answer the question: “Which phases are present?”

Limitations of PDF-2 and databases required for advanced XRD analysis

PDF-2 is limited to routine phase identification and is not suitable for advanced analyses such as full Rietveld refinement, accurate quantitative phase analysis (QPA), or detailed size/strain and structural modeling. For these applications, **PDF-4+** supports advanced qualitative and quantitative analysis with high-quality crystallographic data, while **PDF-5** extends capability to complex and nanostructured materials. Both databases are required for structure-sensitive and quantitative XRD analysis.

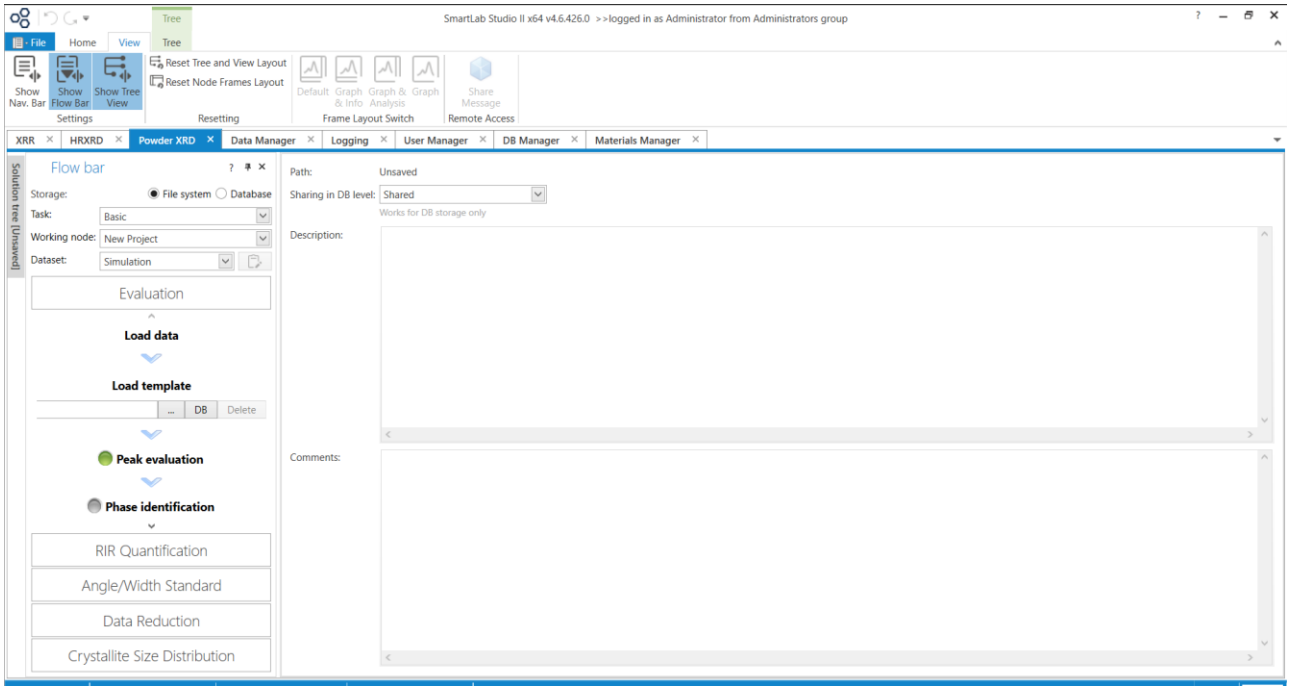
Qualitative Phase Identification Workflow (PDF-2)





Run the SmartLab Studio

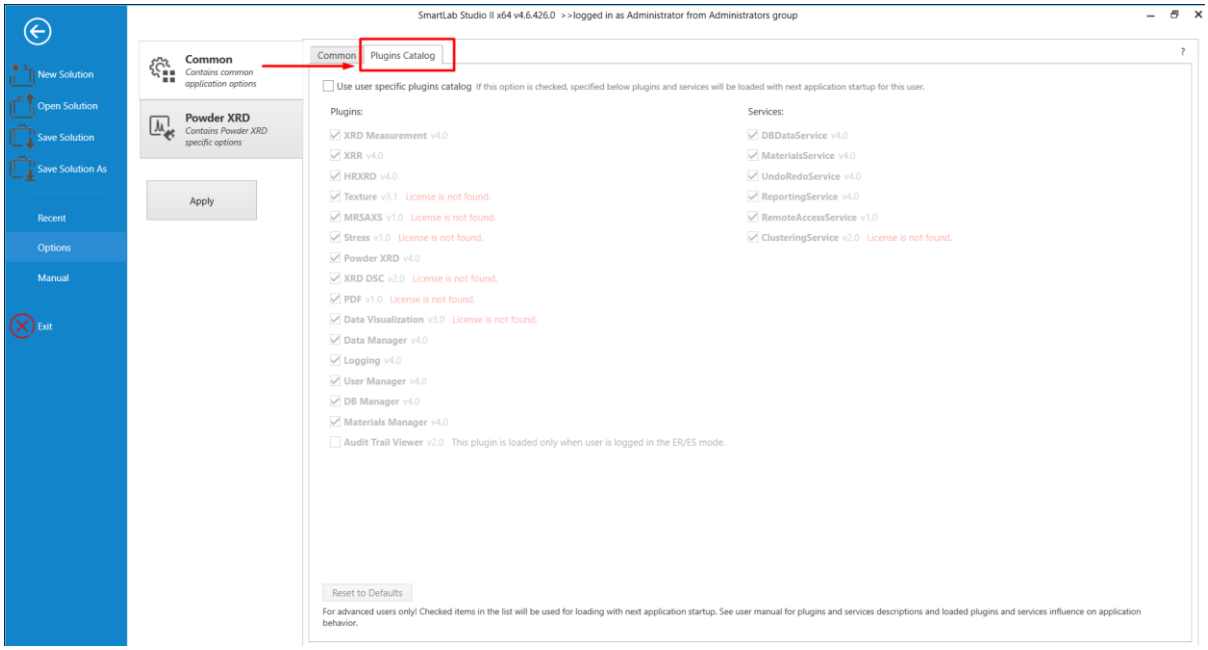
To run the **SmartLab Studio II** double click on the icon



Plugins

To see the **Available Plugins** Click File → Options → Common → Plugin Catelog

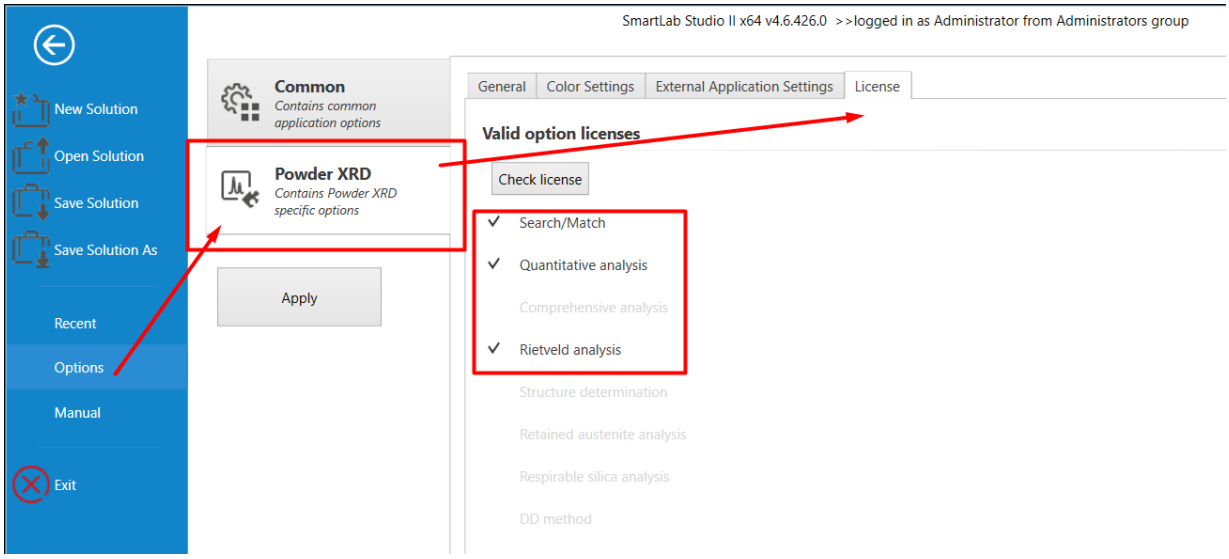
In SmartLab Studio II, a plugin is a modular software component that enables a specific measurement or analysis workflow (e.g., Powder XRD, XRR, HRXRD, residual stress, texture analysis, and data visualization). In the Plugins Catalog, entries labeled “License not found” indicate that the corresponding module is installed or available in the system but is not currently licensed for use.



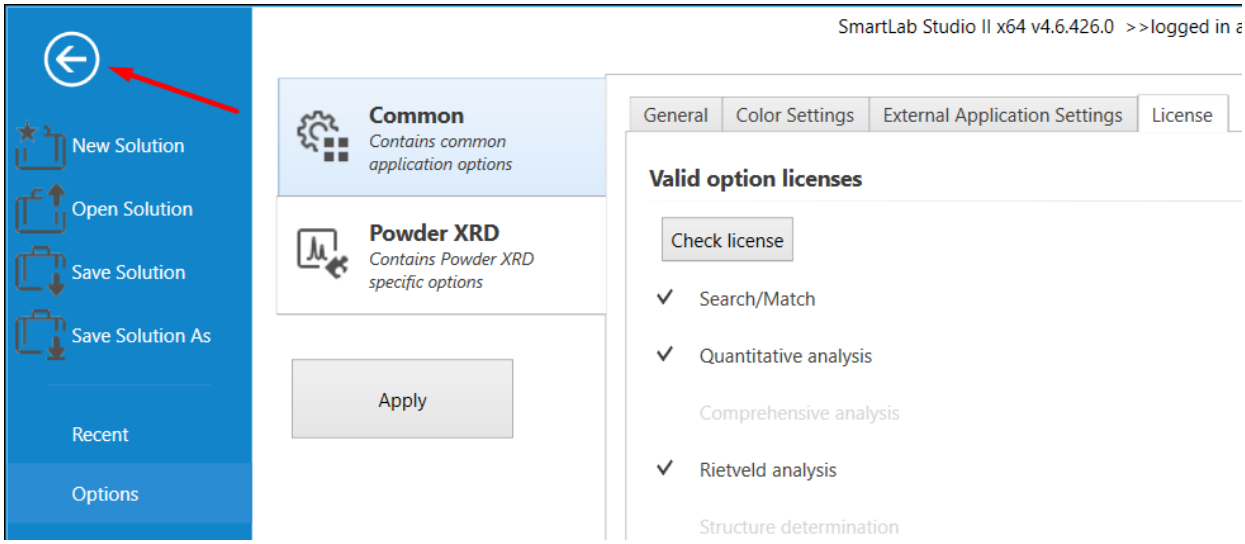
Licenses

To see the **Available Licenses** Click File → Options → Powder XRD → License

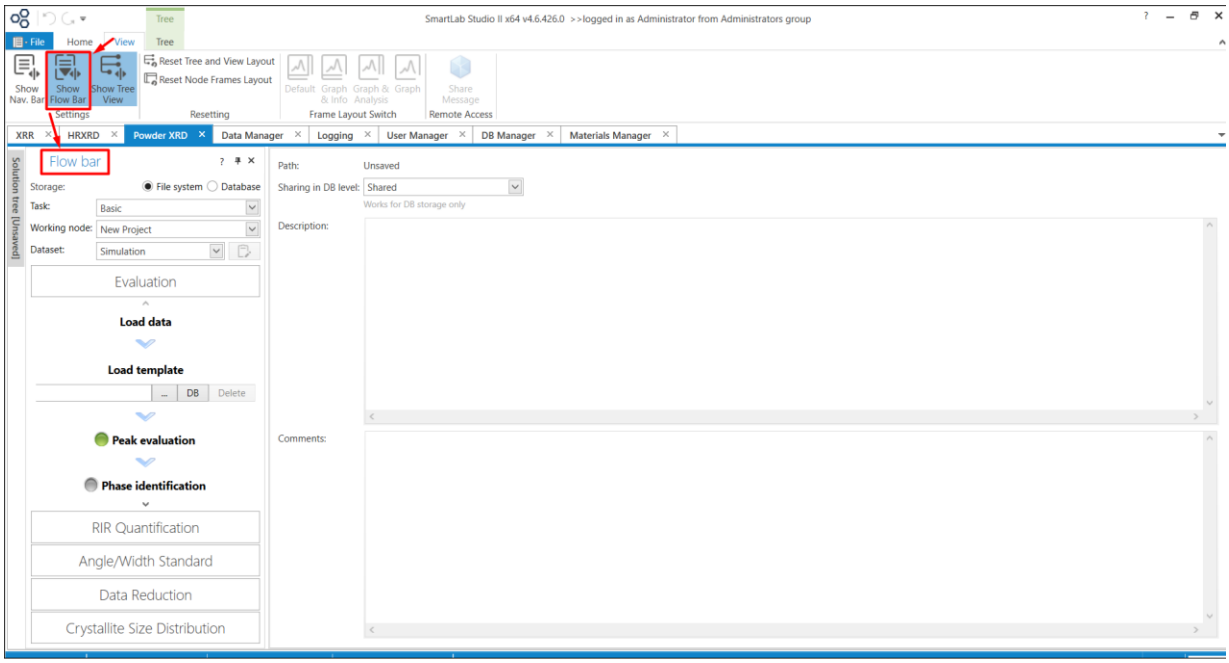
From the Powder XRD option licenses screen (e.g., Search/Match, Quantitative Analysis, and Rietveld Analysis), users can perform phase identification through search/match using an ICDD database such as PDF-2. Functions that are not licensed are displayed as greyed out and cannot be used unless the corresponding option or plugin is added to the active license.



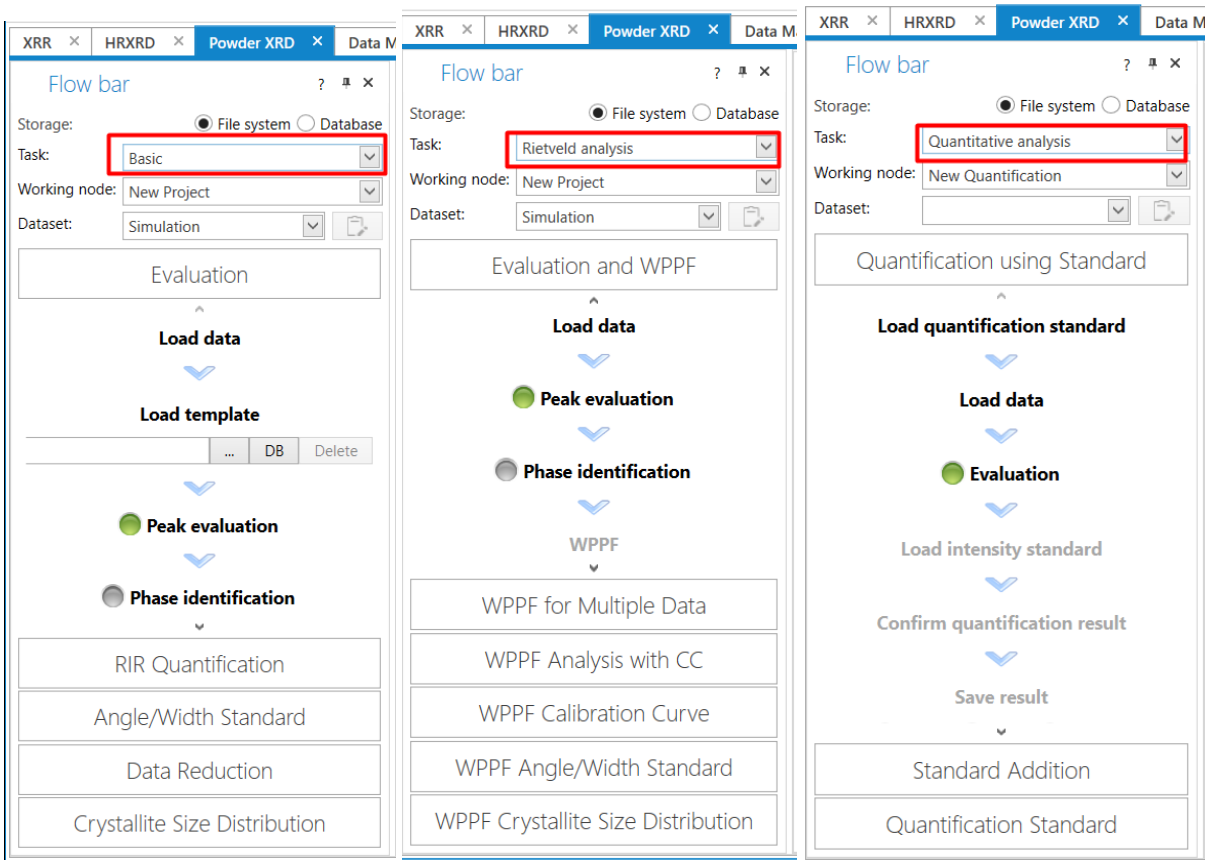
Click back arrow to move back to Powder XRD



Click view → press show flow bar if flow bar is hidden



SmartLab Studio II offers three analysis modes for powder XRD data: Basic, Rietveld analysis, and Quantitative analysis. This document focuses on the Basic XRD analysis mode; the other two modes will be covered later.



1) Basic (identification of phases)

Used for routine qualitative XRD analysis of powder data. It typically covers data loading, preprocessing, data reduction, peak evaluation, and phase identification (Search/Match). It is ideal when the goal is to identify which crystalline phases are present and to generate a clean peak list. It does not require a full structural model for the phases.

2) Rietveld analysis (quantification + detailed structure refinement)

Rietveld analysis in SmartLab Studio II is a whole-pattern refinement method performed under the WPPF (Whole Powder Pattern Fitting) workflow, where the entire measured Powder XRD pattern is fitted using a complete crystallographic structure model (e.g., a CIF file or structural data from PDF-4/PDF-5 containing atomic coordinates and space group information). The software iteratively refines phase fractions, lattice parameters, peak profile shape and width, background, preferred orientation, and microstructural broadening; atomic positions and occupancies may also be refined when data quality and structural reliability allow. This method is selected when accurate quantitative phase analysis and detailed structural characterization are required, and it is considered the standard approach for robust powder diffraction analysis when full structural information is available.

3) Quantitative analysis

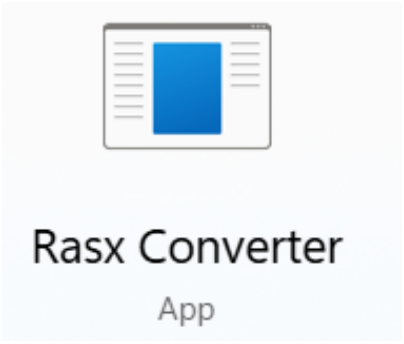
Quantitative analysis in SmartLab Studio II is performed under the “Quantification using Standard” workflow to estimate phase amounts without conducting a full Rietveld (WPPF) refinement. This approach typically applies methods such as RIR (Reference Intensity Ratio) or calibration using external or internal standards, based on previously identified phases and their

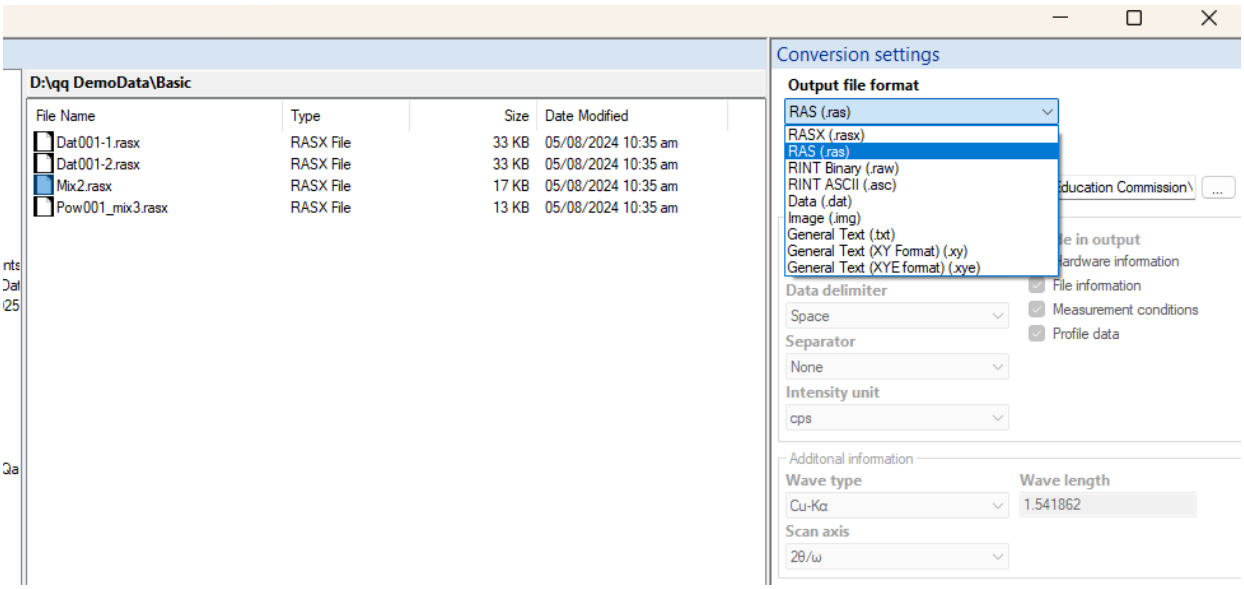
reference intensity data (e.g., from PDF databases). The procedure involves loading a quantification standard, evaluating selected diffraction peaks, and confirming results through intensity normalization. It is suitable for rapid and practical phase quantification when detailed structural refinement is not required. However, the reliability of the results strongly depends on proper sample preparation, accurate peak selection, instrumental stability, and the quality of the reference intensity data used.

Supported file formats and Rasx Converter

These file formats are allowed in SmartLab Studio II.

RUN Rasx Converter to convert a file format





Meaning:

- .rasx → Rigaku SmartLab native format (recommended)
- .ras → Older Rigaku format
- .rad → Rigaku data format (often raw scans)
- .raw → Raw data format

- .asc → ASCII format (intensity vs. 2θ)
- .xy → Generic X-Y data format
- .txt → Text format (must have correct columns)
- .img → Image data (used for 2D detectors, NOT a simple picture like .jpg or .png)

Important Note on .img

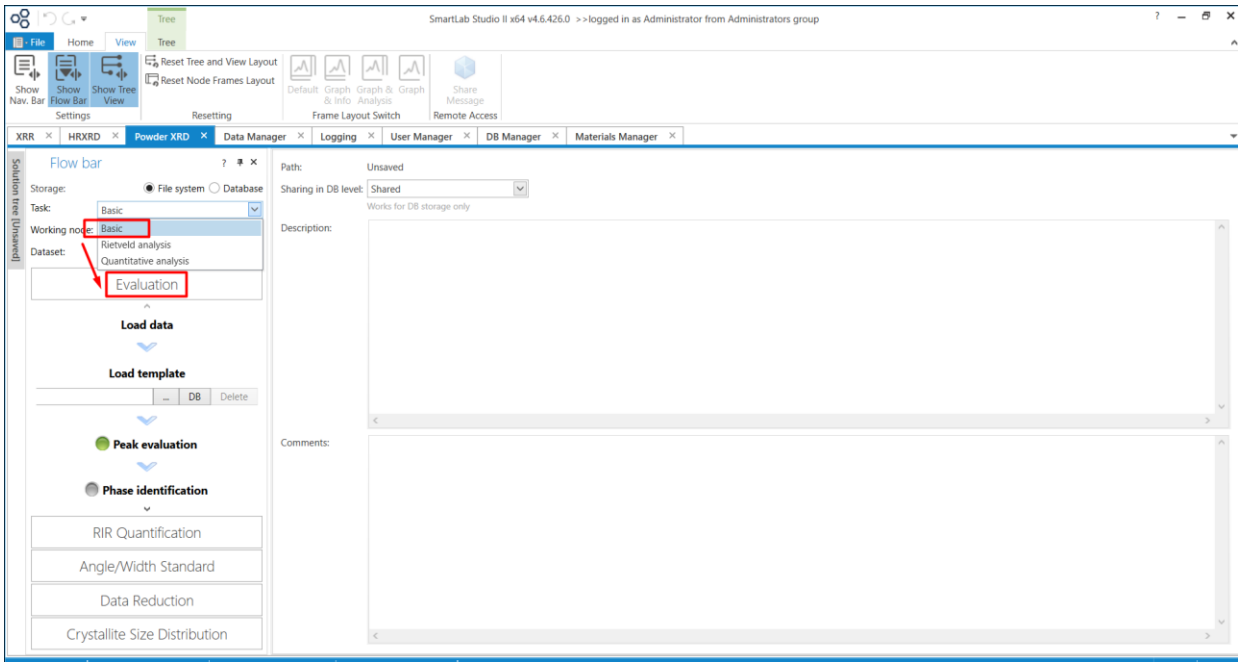
This is not a standard image file (e.g., JPEG or PNG); it is raw 2D diffraction data from the HyPix-3000 detector. Screenshots or photographs cannot be used for analysis in SmartLab Studio II.

Peak Evaluation

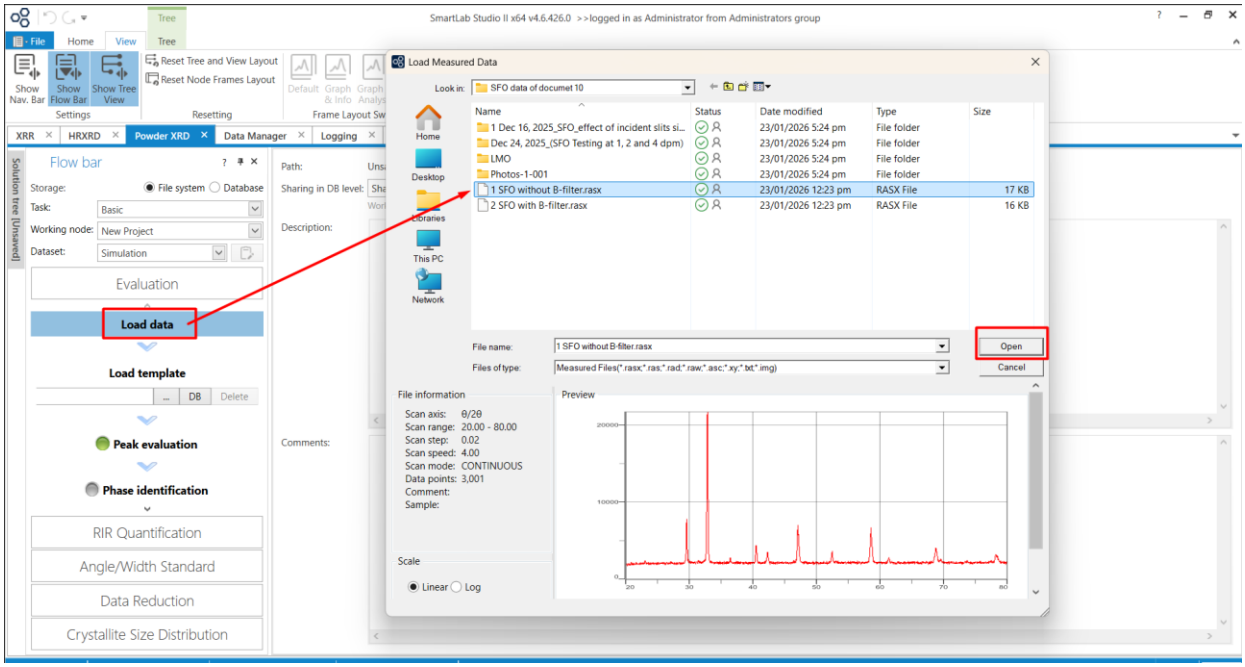
Peak Evaluation is the first essential step in XRD data analysis because it converts the measured diffractogram into a reliable set of peak parameters for interpretation. During data loading, SmartLab Studio II typically performs an automatic evaluation by detecting peak positions (2θ), intensities, widths (FWHM), and background. However, automatic routines can miss very weak reflections, merge overlapped peaks, or mistakenly pick noise/artifacts as peaks especially when the background is high or the data are noisy.

In such cases, manual peak editing is required to add real missing peaks, remove false peaks, and correct peak parameters so the peak list truly represents the measured pattern. After manual changes, a fitting/refinement step should be run to update the peak model and background, ensuring the calculated profile remains consistent with the measured data. Accurate peak evaluation is critical because phase identification and any further analysis depend directly on the quality of the peak list.

Select Basic → Select Evaluation

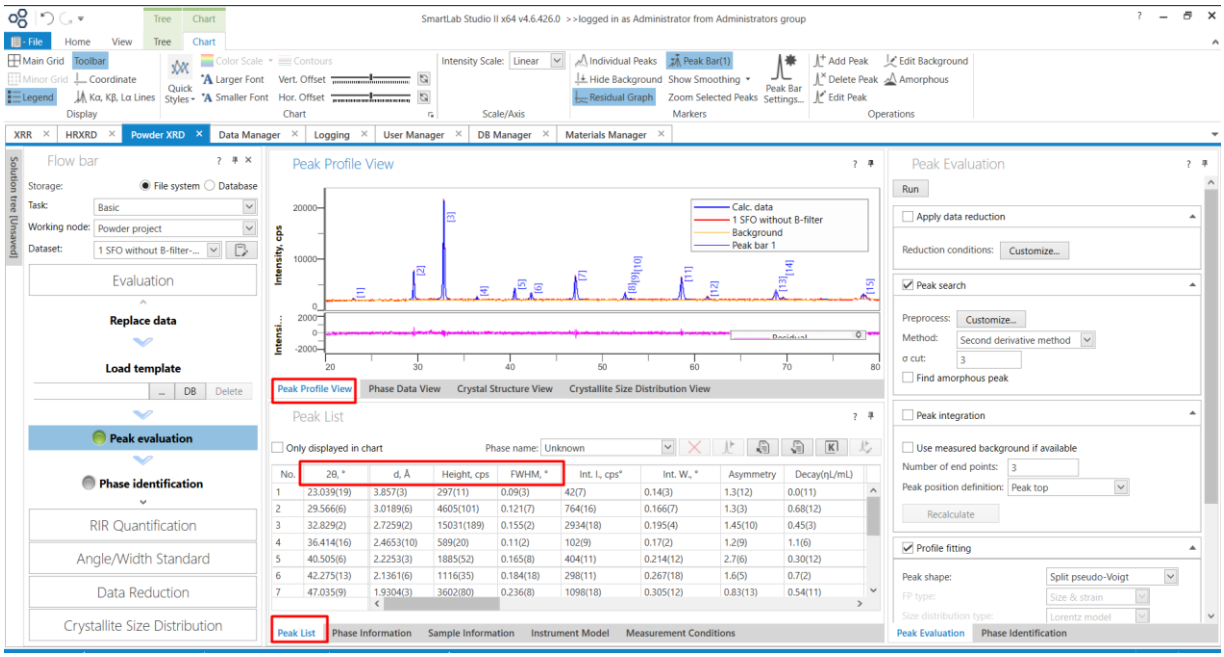


First, load the measurement data. As the data is being loaded, the software automatically performs peak evaluation.

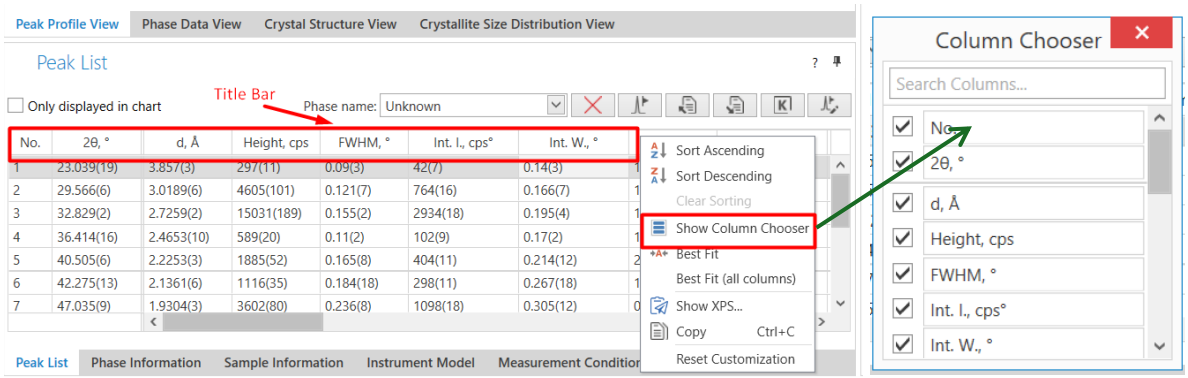


After data is loaded, the Load data button in the Flow bar changes to Replace data. Clicking Replace data loads new data while keeping the current analysis settings unchanged.

During the evaluation process, parameters such as 2θ, d-spacing, peak height, FWHM, and others are calculated automatically



Right-click the title bar and select Show Column Chooser to add or remove items from the display.

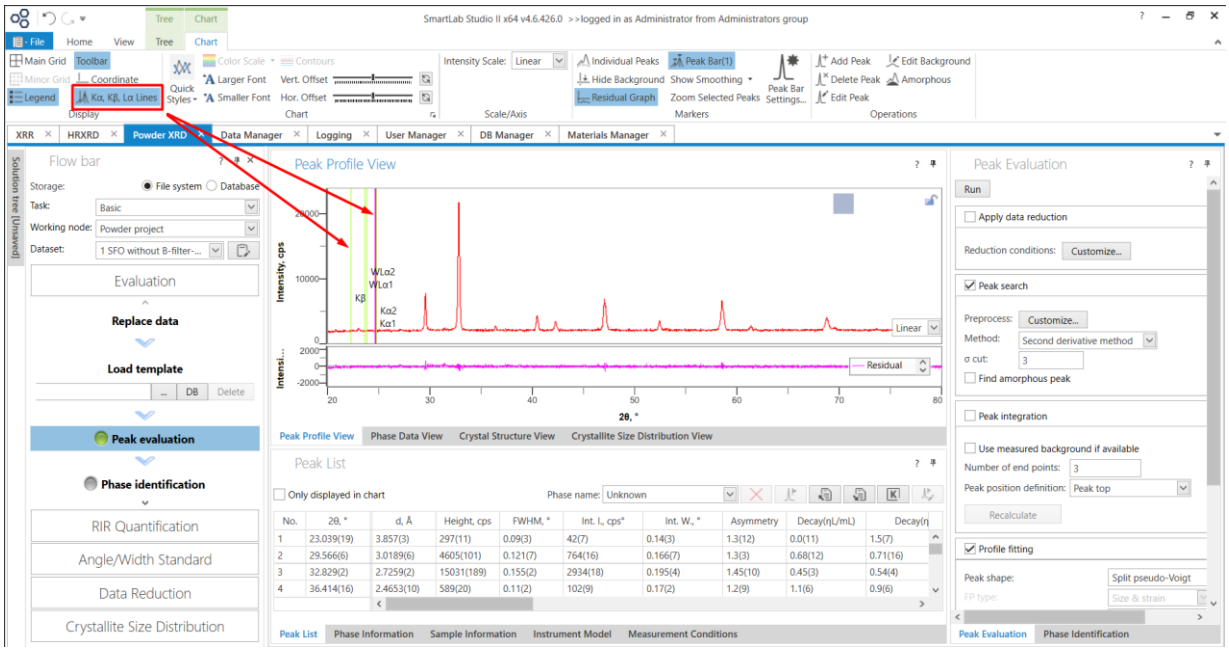


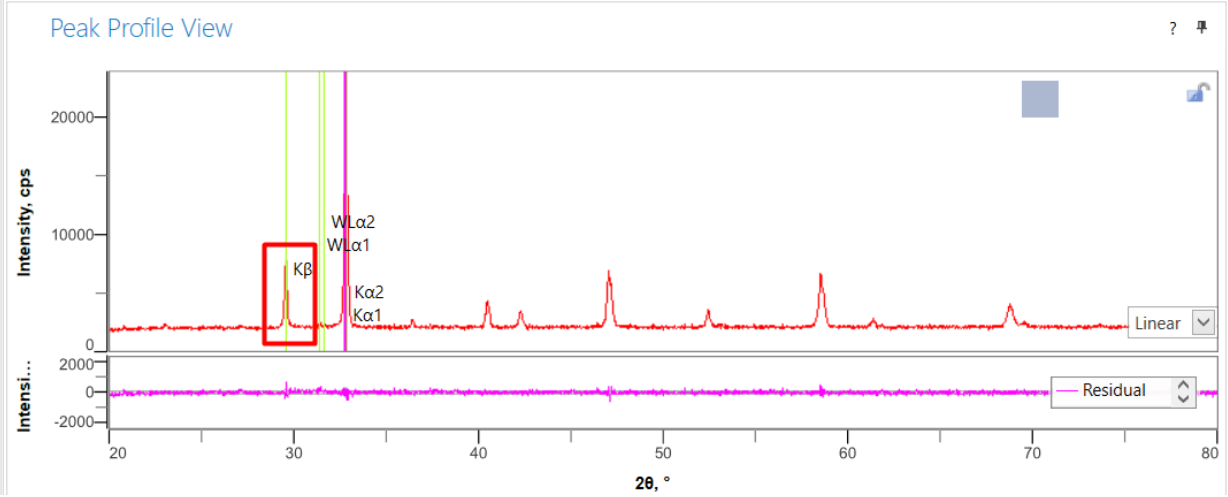
K-Beta Peak Identification

Some diffraction peaks may originate from Kβ radiation rather than actual crystalline phases, and retaining them can lead to incorrect phase identification, as this peak will interfere with the qualitative analysis and should be deleted. To verify whether a peak is due to Kβ radiation, use the Show Kα, Kβ, and Lα Lines cursor option in the Powder XRD toolbar.

When this function is enabled, the Kα1 marker appears in pink, while the Kβ marker appears in green. Align the pink Kα1 marker with a strong diffraction peak, then check whether any nearby peak coincides with the green Kβ position. Any peak that overlaps with the Kβ position is a Kβ-derived artifact and should be deleted before performing qualitative analysis, as these peaks may cause false matches during phase identification.

Repeat this check for all major peaks in the profile. Once all Kβ-related peaks have been removed and peak evaluation is complete, click Refine under *Profile Fitting* to proceed with the analysis.




Peak Profile View
Intensity, cps
20000
10000
0
WLα2
WLα1
Kβ
Kα2
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2000
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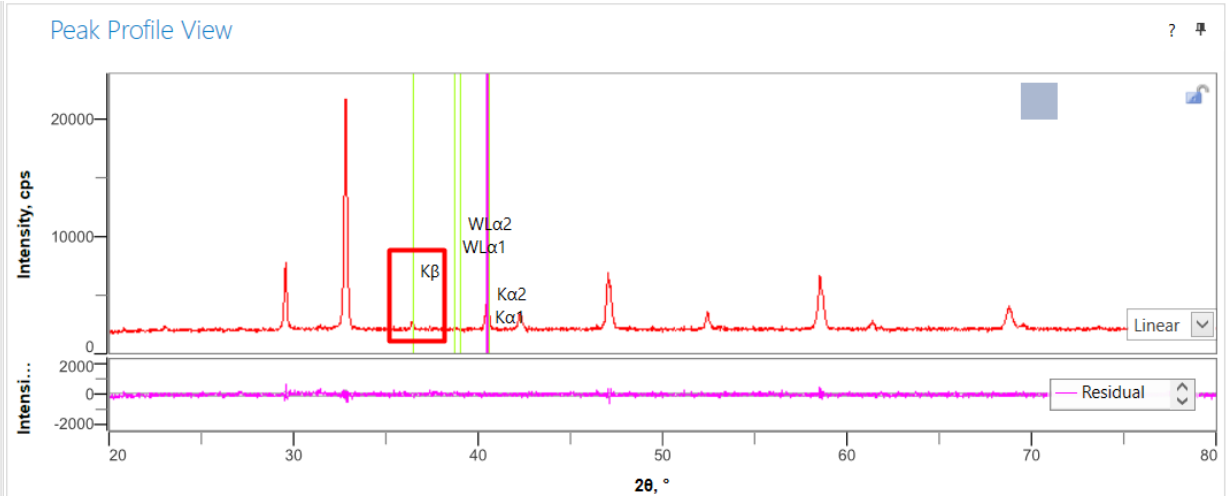
Peak Profile View
Intensity, cps
20000
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WLα2
WLα1
Kβ
Kα2
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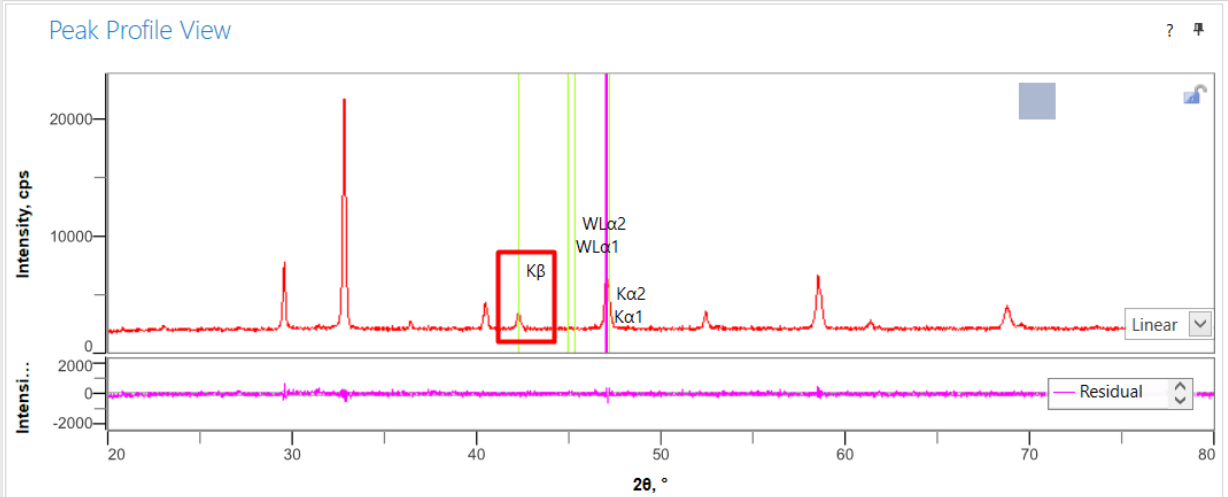
2θ, °


Peak Profile View
Intensity, cps
20000
10000
0
WLα2
WLα1
Kβ
Kα2
Kα1
Linear
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Residual
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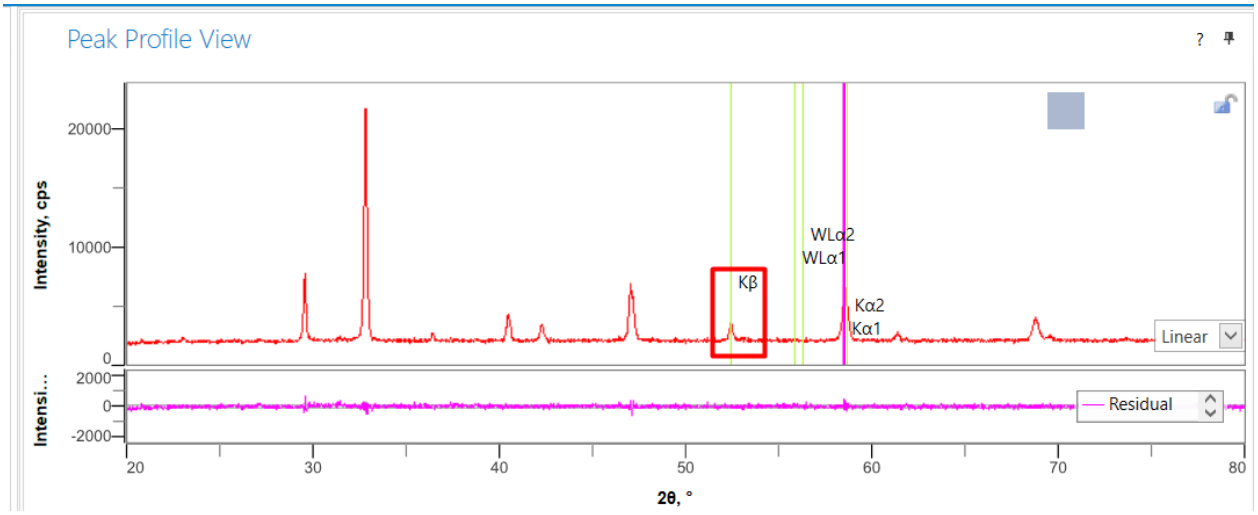
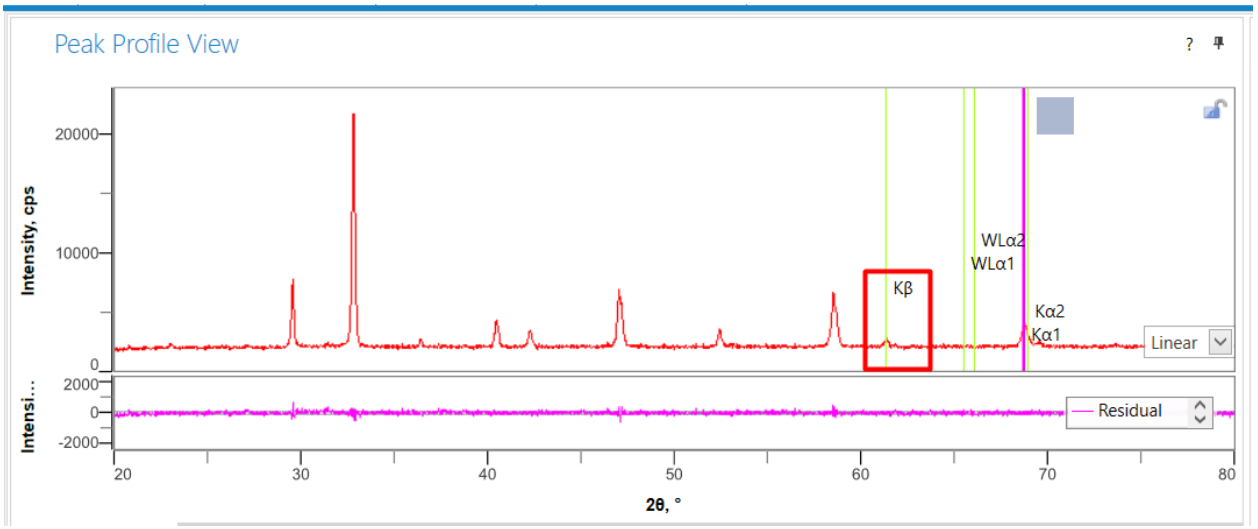
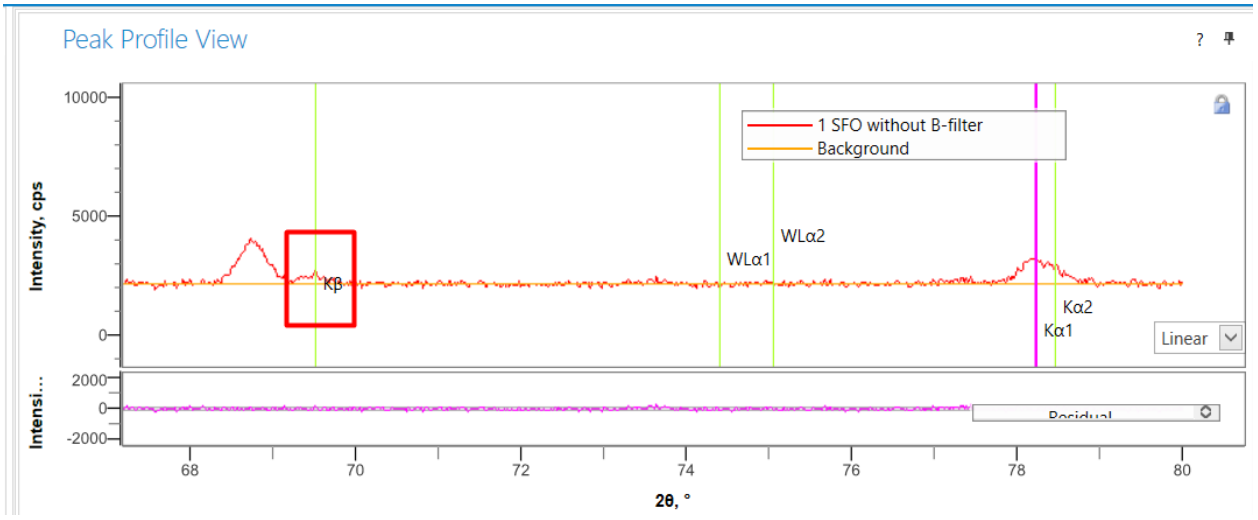
2θ, °



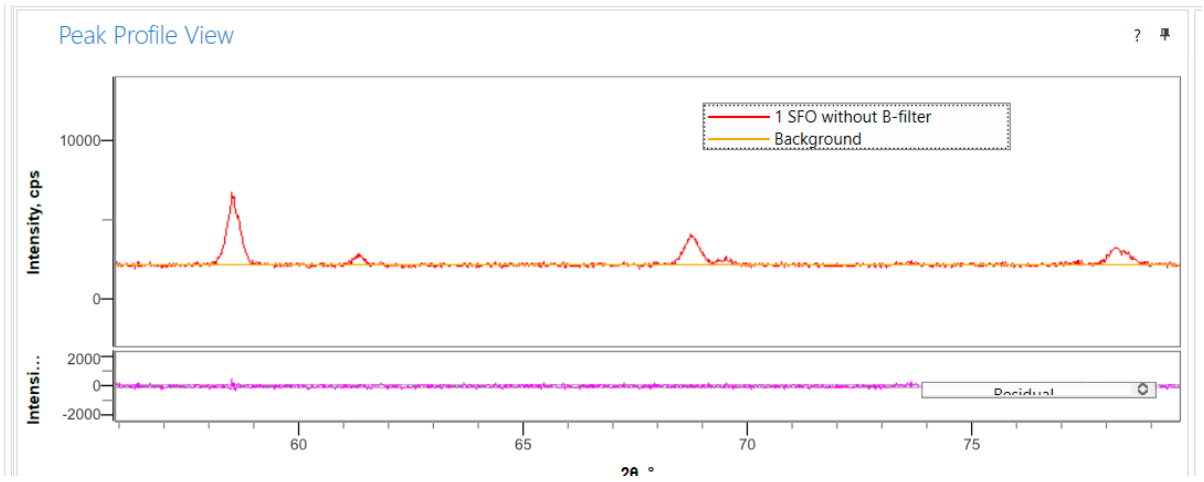




Once finished uncheck the Show Kα, Kβ, and Lα lines.

You can Zoom in by left-clicking and dragging to draw a selection box. To view the other part of the chart, right-clicking and drag the chart.

You will see the zoom in view

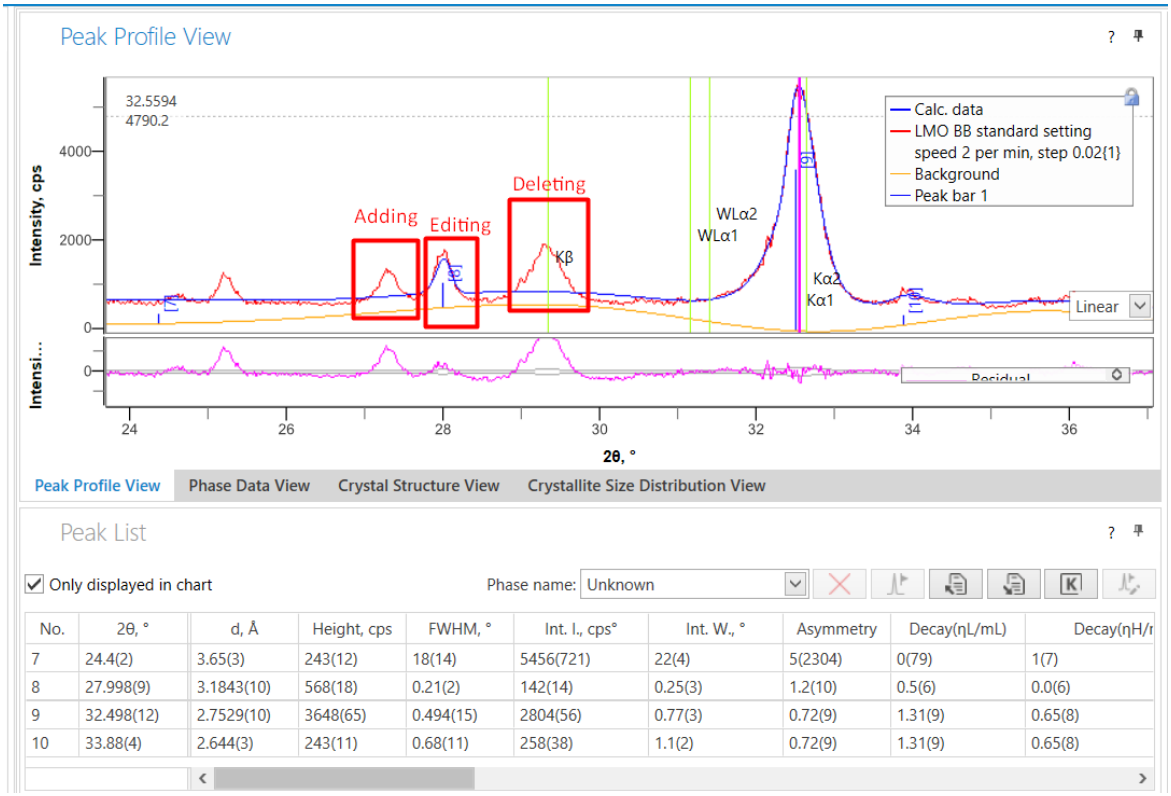


Right click on the chart and click Reset view

Adding, Editing and Deleting Peaks

Peak evaluation is performed automatically when the measurement data is loaded, but manual adjustments may still be necessary because accurate peak identification is essential. Automatic detection may miss small or weak peaks or may not perfectly match the measured profile. In such cases, you should manually refine the peak list to eliminate discrepancies between the

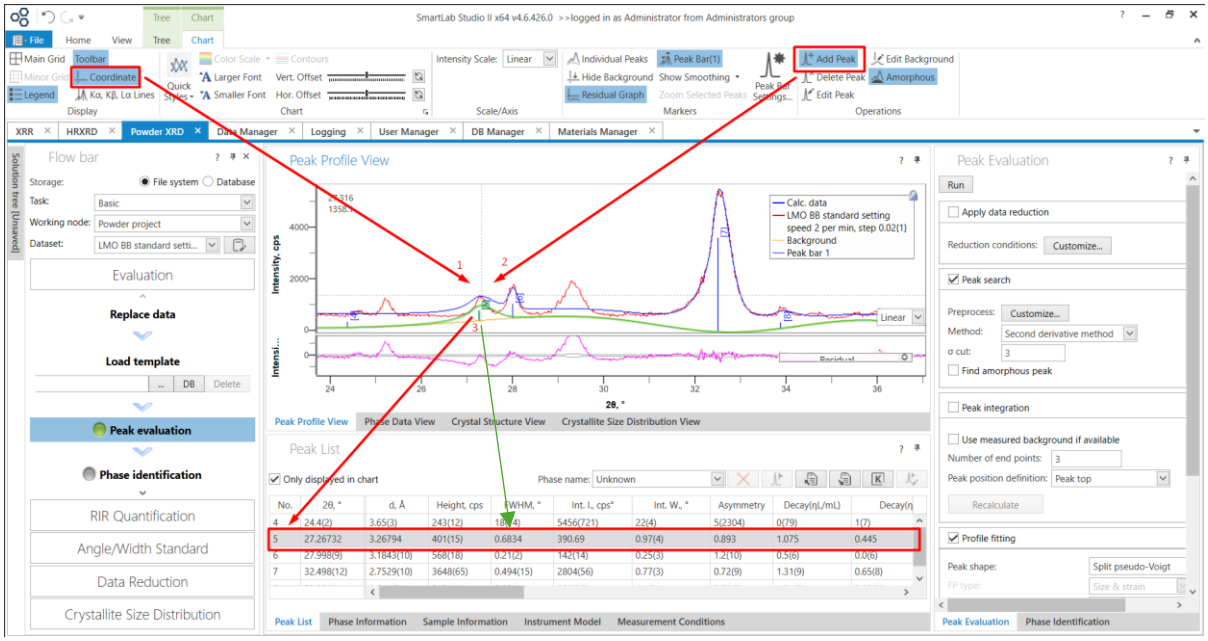
measured and calculated data. If any peaks are missing, they can be added using the “Add Peak” option. Likewise, existing peaks can be edited or deleted as needed to achieve an accurate representation of the diffraction pattern.



No.	2θ, °	d, Å	Height, cps	FWHM, °	Int. I., cps°	Int. W., °	Asymmetry	Decay(ηL/mL)	Decay(ηH/r
7	24.4(2)	3.65(3)	243(12)	18(14)	5456(721)	22(4)	5(2304)	0(79)	1(7)
8	27.998(9)	3.1843(10)	568(18)	0.21(2)	142(14)	0.25(3)	1.2(10)	0.5(6)	0.0(6)
9	32.498(12)	2.7529(10)	3648(65)	0.494(15)	2804(56)	0.77(3)	0.72(9)	1.31(9)	0.65(8)
10	33.88(4)	2.644(3)	243(11)	0.68(11)	258(38)	1.1(2)	0.72(9)	1.31(9)	0.65(8)

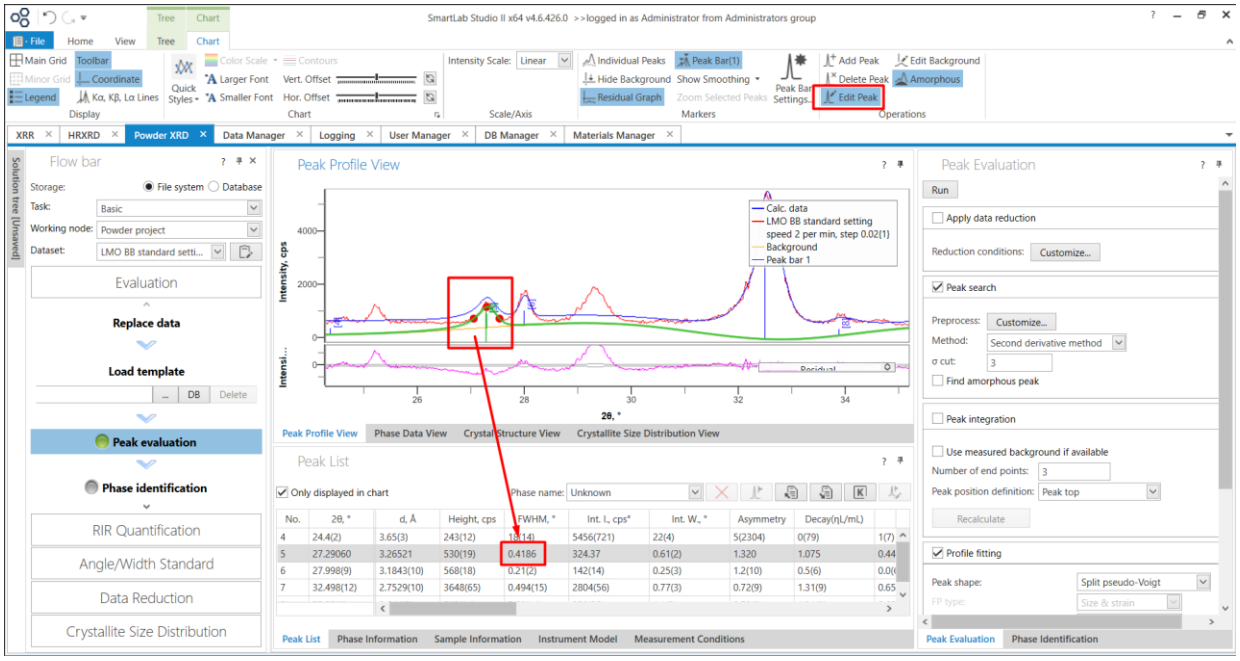
Adding Peaks

Although peak evaluation is performed automatically, small peaks may sometimes be missed or incorrectly processed. In such cases, manually adding the missing peaks ensures accurate peak determination. After manually adding the necessary peaks, repeat the refinement process to ensure proper evaluation of any peaks that were missed.

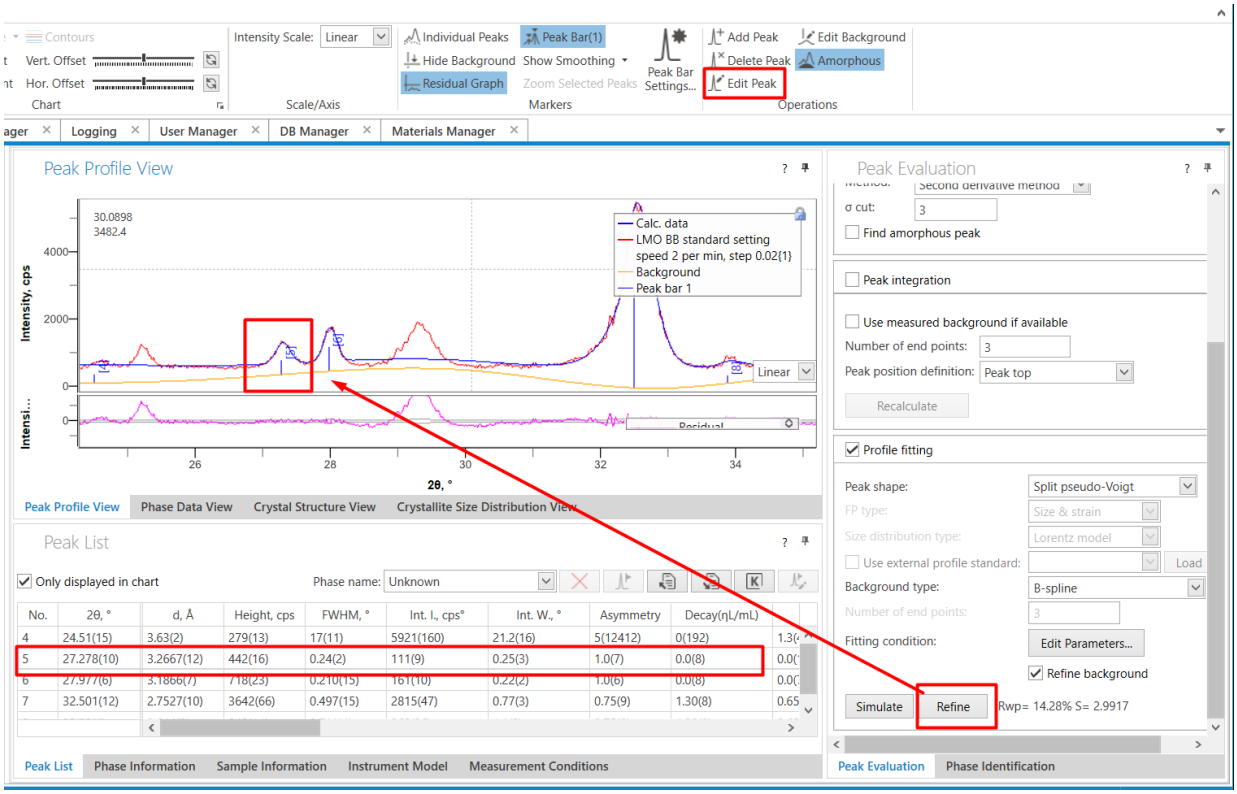


Editing Peaks

Peaks can be modified using Edit Peak and clicking the target peak. The left and right red markers adjust the peak width and shape, while the middle red marker changes the peak height. The green line is used to adjust the position of the peak along the graph. By carefully adjusting these markers, by moving these markers carefully, the peak can be fitted more accurately to the measured data.

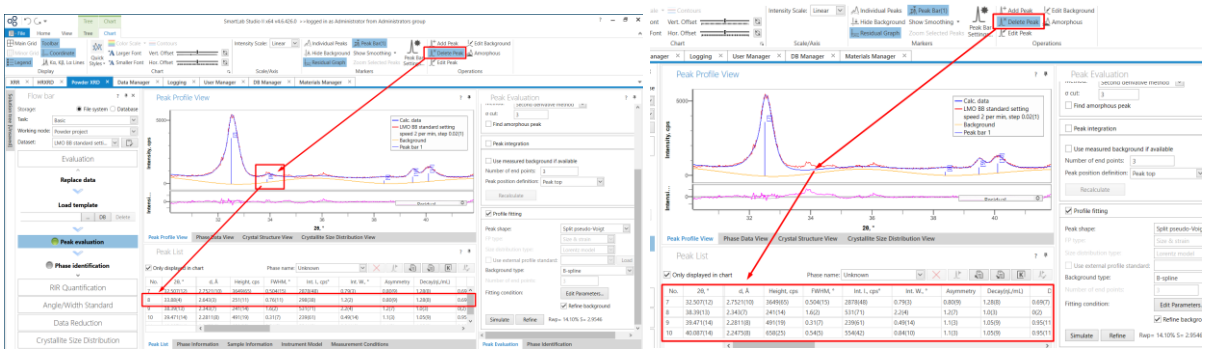


After completing all edits, click Refine under *Profile Fitting* to update the peak evaluation.

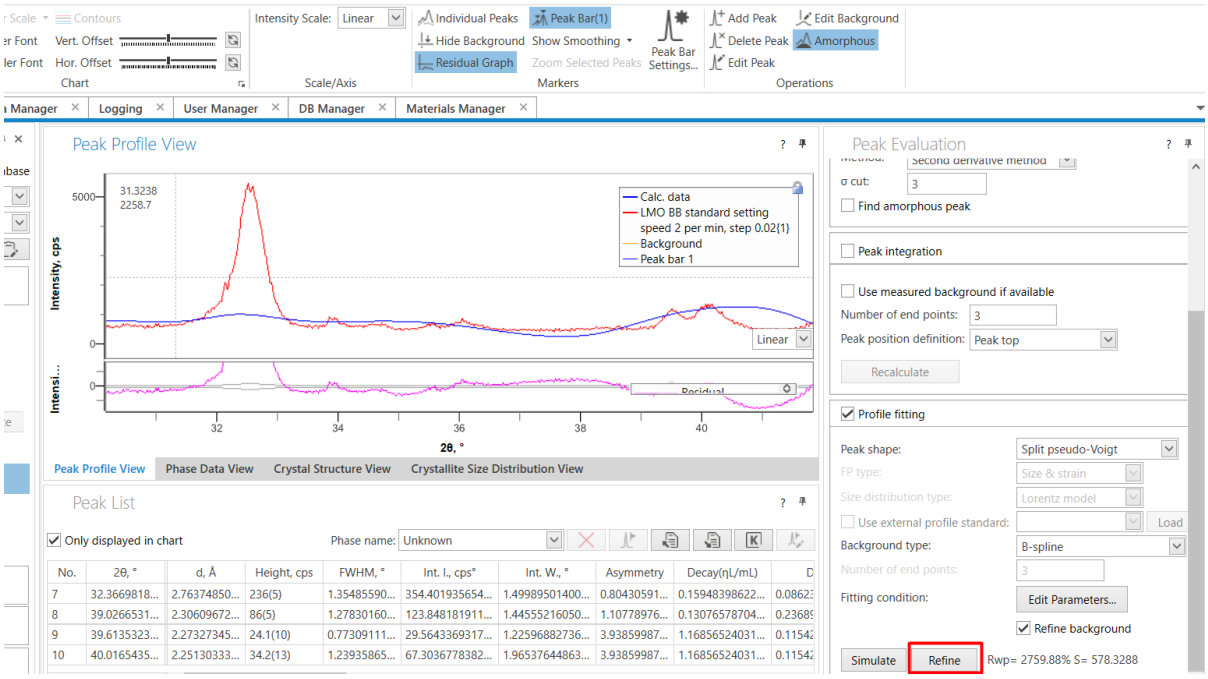


Deleting Peaks

If noise is mistakenly detected as a peak, remove it using Delete Peak. Automatic peak evaluation can sometimes identify noise as real peaks, so such peaks must be deleted manually to maintain accuracy.



After deleting any incorrect peaks, refine the calculated data to ensure proper fitting, following the same procedure used when adding a peak.

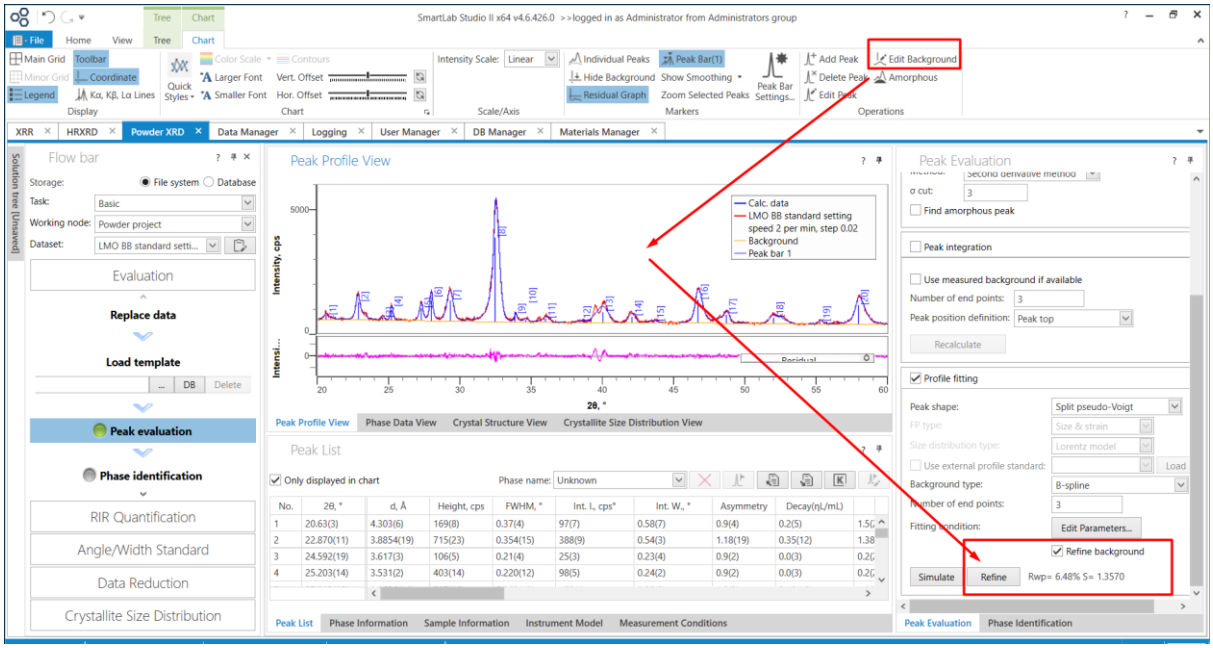


Background Editing

In XRD, the background is the slowly varying intensity baseline beneath the Bragg peaks, arising from non-Bragg contributions such as air scatter, incoherent/Compton scattering, sample fluorescence (often significant for Cu Kα with Fe/Co/Ni-bearing samples), diffuse scattering from disorder, peak tails, and sometimes broad features from amorphous material or very small crystallites; in SmartLab Studio II, background editing means fitting/adjusting this baseline (using background markers/points) so it follows the *true* underlying signal and can be appropriately subtracted for cleaner peak evaluation. Manual editing is needed when the automatically calculated background is sloped, curved, elevated, noisy, or distorted, because an incorrect baseline can be mistaken as part of peaks and lead to inaccurate peak heights, areas, and

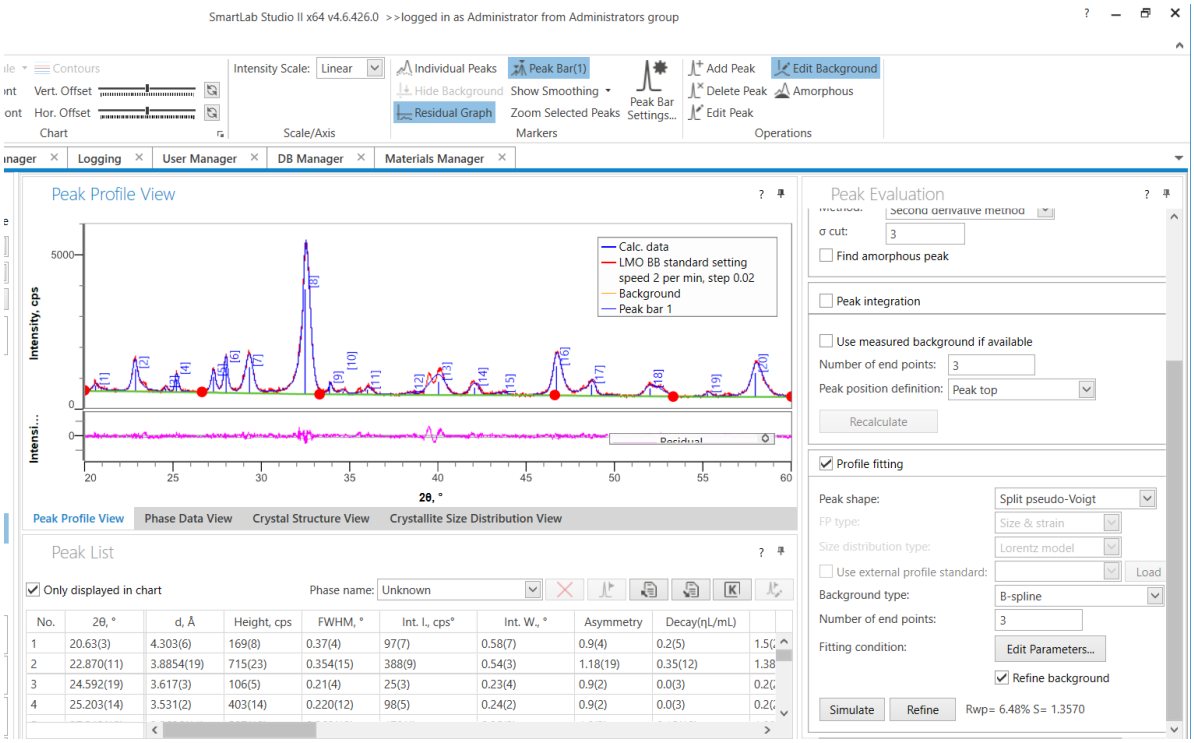
FWHM, causing missed/merged weak peaks and unreliable phase identification. Correct background editing improves peak-to-background ratio, stabilizes peak finding and profile fitting, and increases the reliability of qualitative and quantitative analyses (including phase ID and Rietveld), but it must be applied conservatively over-subtraction can remove real weak peaks, distort intensity ratios used in search–match, flatten genuine amorphous humps, or even produce negative intensities, which may result in incorrect or missed phases.

When Edit Background is selected, red markers appear on the graph. These markers define the background shape, and you can adjust them by dragging the markers so that the background curve follows the measured data accurately. Additional markers can be added by Ctrl + clicking on the profile, and existing markers can be deleted by Ctrl + clicking on the marker itself. These red markers act as nodes used to calculate the background intensity. Adjust or add/delete nodes as needed until the background line closely matches the measured pattern. Once the background shape is satisfactory, click Refine under *Profile Fitting* to apply the changes. If you want to preserve the manually adjusted background without automatic modifications, make sure to uncheck “Refine Background” before refining.



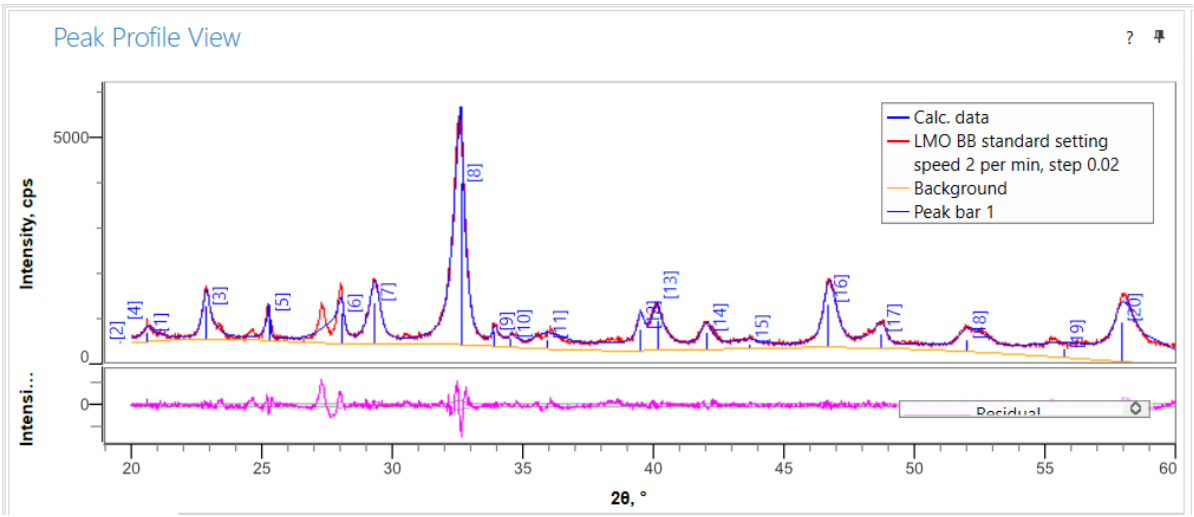
A correctly fitted background helps achieve:

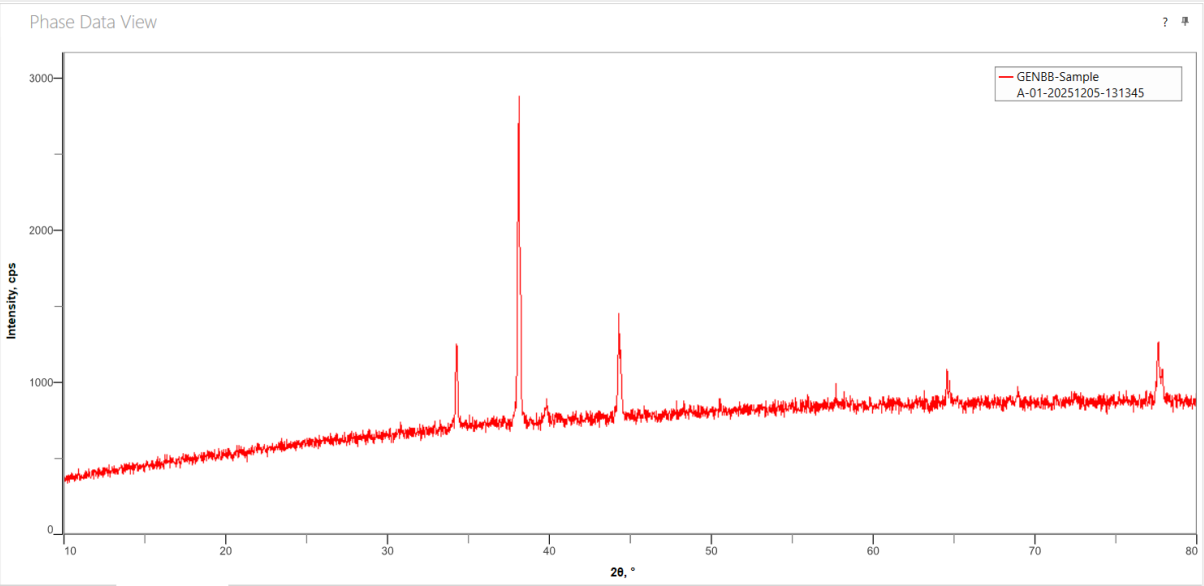
- Accurate peak intensities (height and, more importantly, integrated area)
- More reliable FWHM/peak-shape parameters (less bias from baseline errors)
- More reliable qualitative phase identification (especially for weak/minor phases)
- More stable quantitative analysis (Rietveld/profile fitting) with fewer systematic residual



✓ Check “Refine Background” when you want the software to automatically smooth and optimize the background after your manual adjustments.

✓ Uncheck “Refine Background” when your manually set background is accurate and you want to keep it fixed without any automatic modification during refinement.





For routine phase identification and profile fitting, the automatic background in this example is acceptable. As a precaution, zoom to 10–25° and 55–80° 2θ and confirm the background curve follows the true inter-peak minima; adjust/add background points only in peak-free valleys and never on peak tails to avoid over-subtraction.

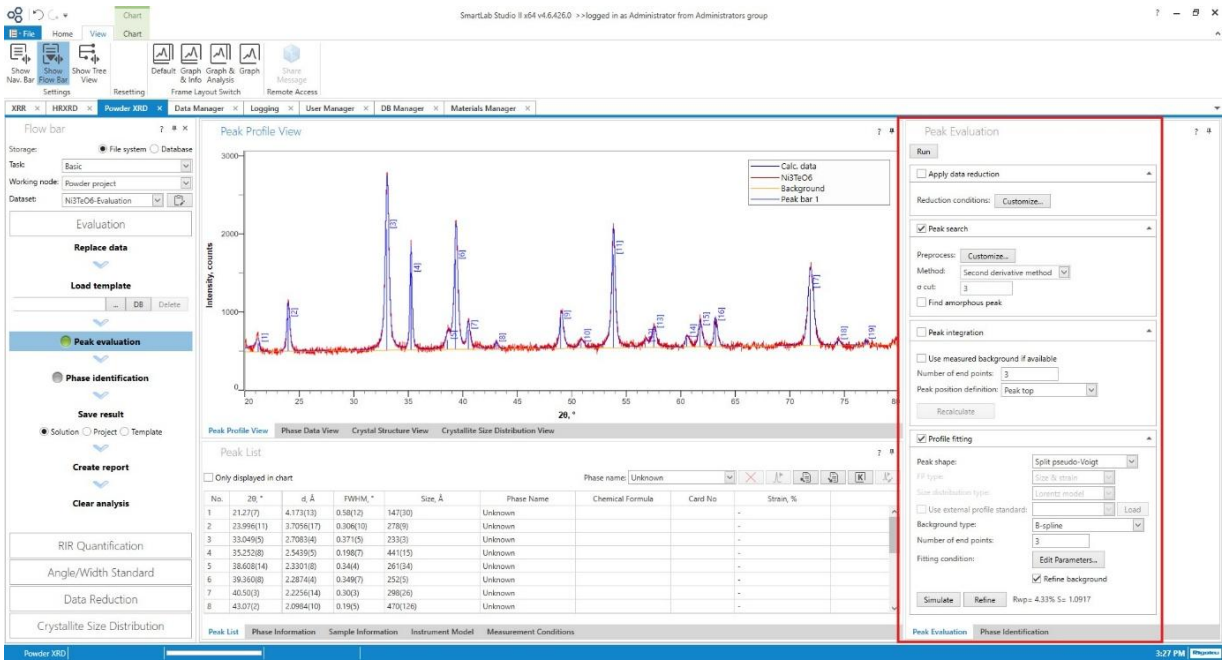
Peak Evaluation: Peak Search, Integration & Profile Fitting

RUN (Peak Evaluation)

What it does: Executes the Peak Evaluation workflow using the options that are currently checked (e.g., Apply data reduction, Peak search, Peak integration, Profile fitting) and then updates the plot, peak markers, and peak list.

When/why to use: Click Run after changing any evaluation setting (σ cut, method, preprocess, reduction conditions, fitting options) or after loading/replacing data, so the software recalculates results with the new parameters.

Effect: It can add/remove/shift peaks if *Peak search* is enabled, and it can update fitted peak parameters/background if *Profile fitting* is enabled so avoid running it with Peak search checked when manual peak edits must be preserved.



Apply data reduction

Applies preprocessing to improve peak visibility (e.g., smoothing, background handling, Kα2 stripping). For qualitative ID, use it to reduce noise and make peak positions clearer, but avoid over-smoothing that can distort weak peaks.

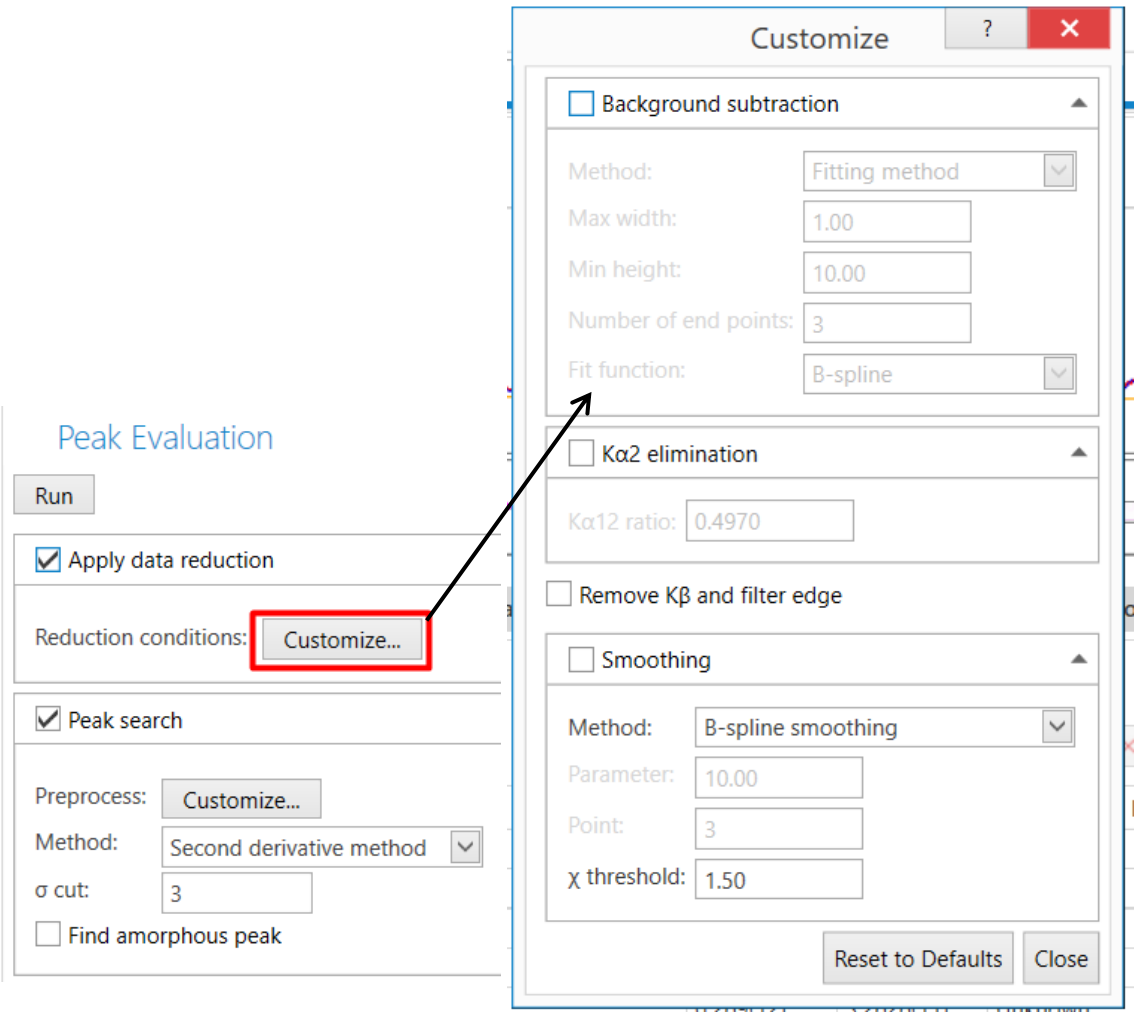
Reduction conditions (Customize…)

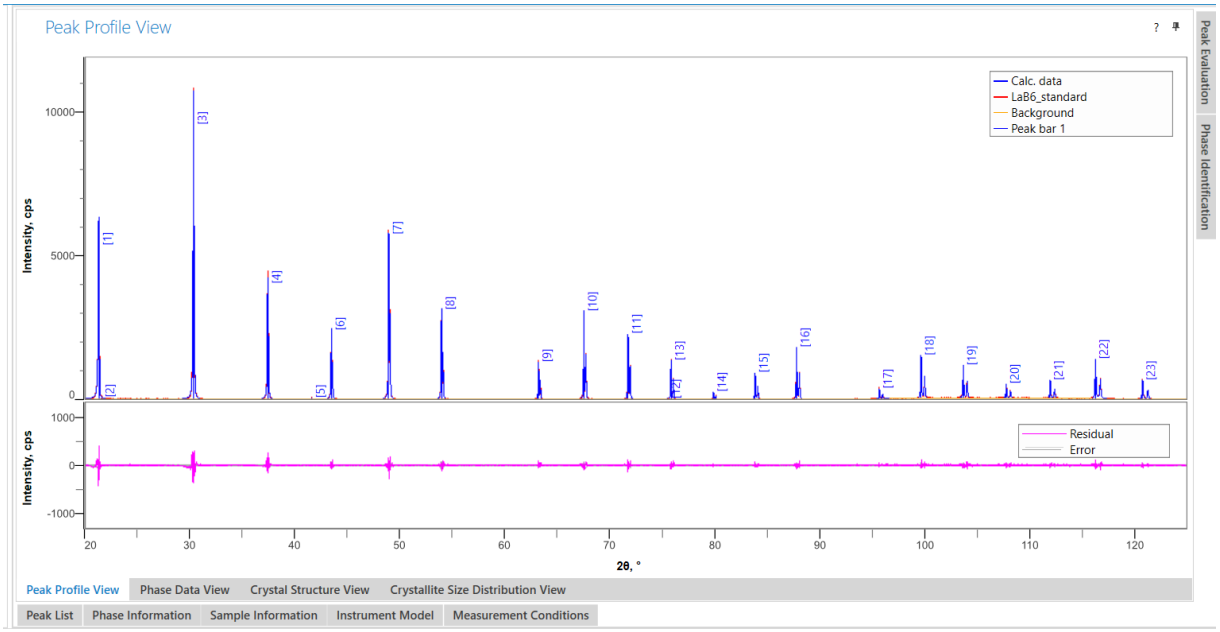
Opens the detailed parameters for data reduction (how much smoothing, background treatment, etc.). Set these to enhance true peaks while keeping peak positions and shapes realistic for database matching.

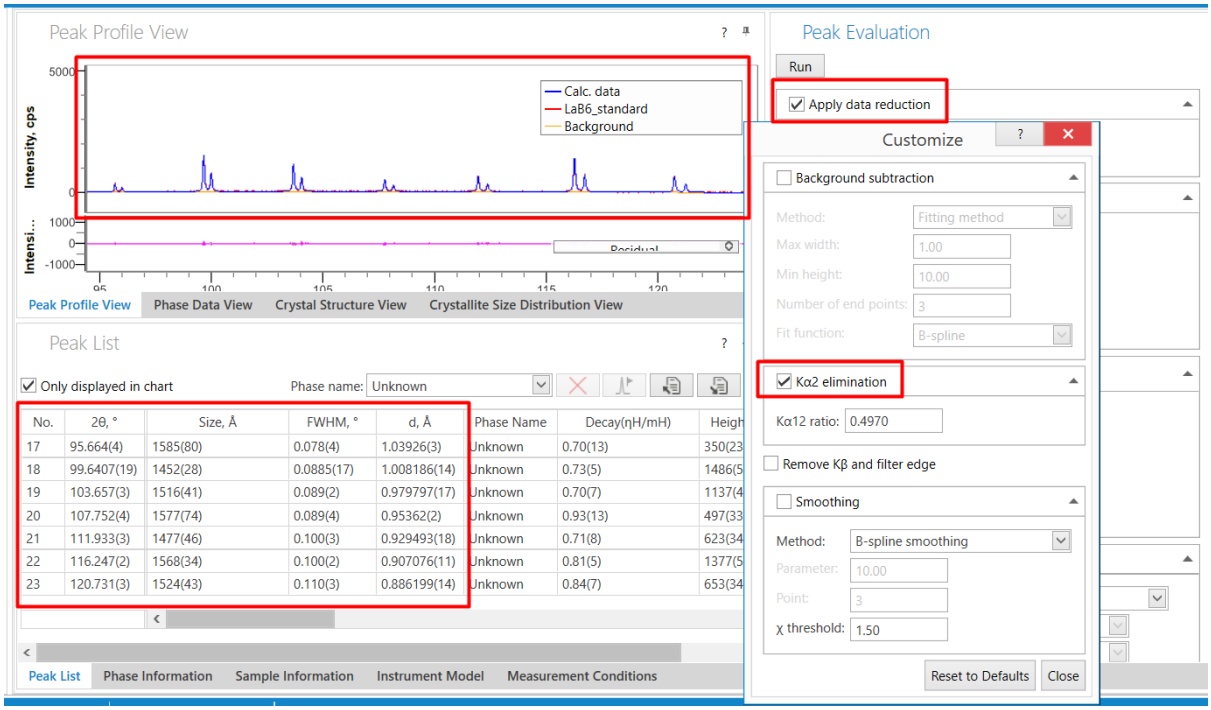
$K\alpha_2$ Elimination (Use vs. Avoid)

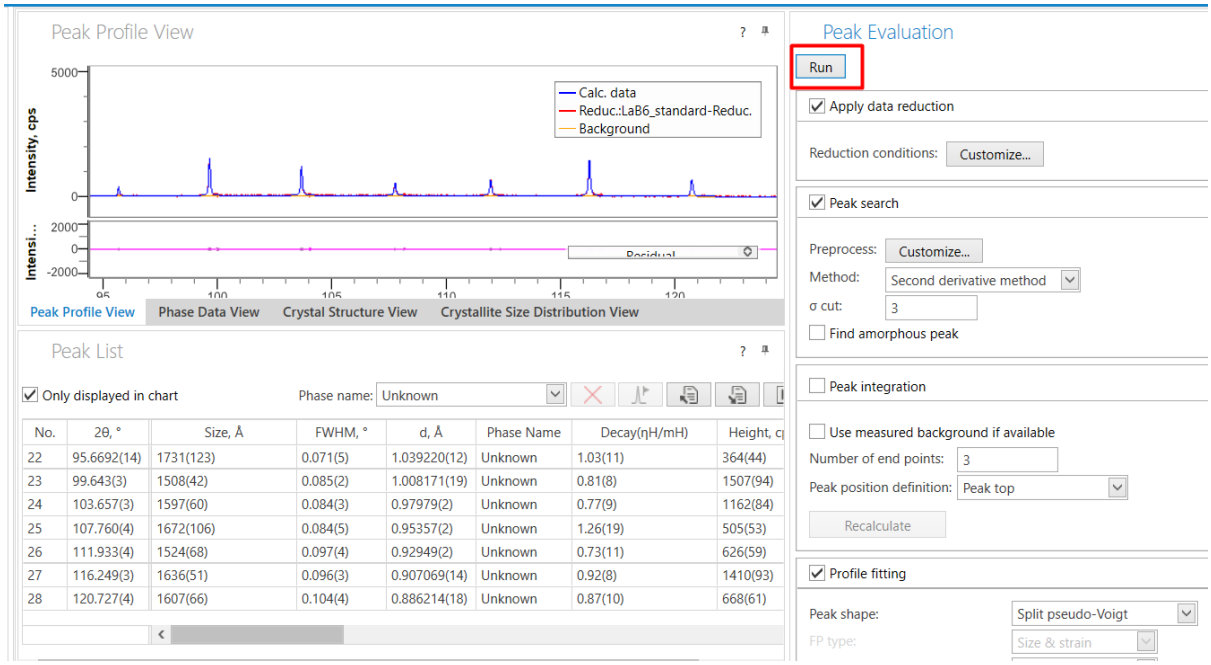
$K\alpha_2$ elimination is suitable for peak picking and qualitative phase ID, because it converts the $K\alpha_1$+$K\alpha_2$ doublet into an approximate single $K\alpha_1$ peak, improving symmetry for search/match and basic fitting. $K\alpha_2$ elimination should be avoided for Rietveld refinement and line-profile/microstructure work, since stripping is a subtraction procedure that can distort profiles, change relative intensities, and amplify noise biasing FWHM/asymmetry/integrated-intensity results unless the workflow is strictly $K\alpha_1$-only.

Because crystallite size calculations depend directly on FWHM, any FWHM change introduced by $K\alpha_2$ elimination will change the reported size so size analysis must use one consistent (stripped or unstripped) workflow throughout.


Peak Evaluation
Run
Apply data reduction
Reduction conditions:
Customize...
Peak search
Preprocess:
Customize...
Method:
Second derivative method
σ cut:
3
Find amorphous peak
Customize
Background subtraction
Method:
Fitting method
Max width:
1.00
Min height:
10.00
Number of end points:
3
Fit function:
B-spline
Kα2 elimination
Kα12 ratio:
0.4970
Remove Kβ and filter edge
Smoothing
Method:
B-spline smoothing
Parameter:
10.00
Point:
3
χ threshold:
1.50
Reset to Defaults
Close

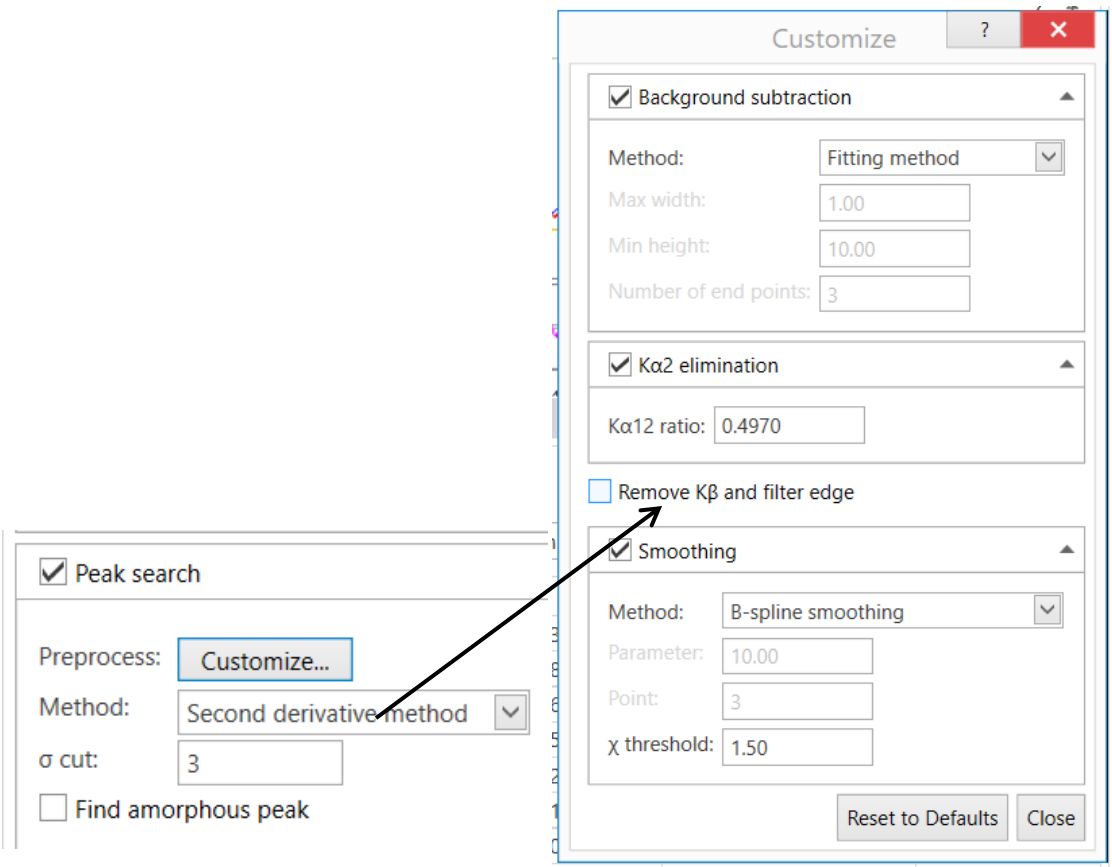

Peak Profile View
Calc. data
LaB6_standard
Background
Peak bar 1
Residual
Error
Intensity, cps
2θ, °
Peak Profile View
Phase Data View
Crystal Structure View
Crystallite Size Distribution View
Peak List
Phase Information
Sample Information
Instrument Model
Measurement Conditions
Peak Evaluation
Phase Identification





Peak search

Automatically detects peaks and populates the peak list used for phase matching. For qualitative ID, this is the main tool to generate the initial peak list before manual cleanup (add/remove/edit).



Preprocess (Customize...)

Controls optional preprocessing applied *specifically for peak finding* (often additional smoothing/derivatives). Useful when peaks are noisy or weak, but too much preprocessing can create false peaks or shift peak tops.

Method (Peak top method)

The Peak top method identifies peaks by searching for local intensity maxima in the measured XRD pattern: a peak is reported when the intensity rises above the surrounding baseline/noise and reaches a clear "top" that satisfies the set detection threshold (e.g., σ-cut). This method is fast, stable, and easy to interpret, making it well suited for routine phase identification when peaks are strong, sharp, and well separated. Its main limitation is that it can miss weak or broad peaks, and it may merge overlapping peaks or ignore shoulders, because it relies primarily on the presence of a distinct maximum.

Method (e.g., Second derivative method)

This method finds peaks by looking at the shape (curvature) of the XRD curve, not just how tall a peak is. It marks a peak where the curve bends strongly in a "peak-like" way, so it can detect small or hidden peaks that do not have a clear top. This method is particularly useful for weak peaks, broad peaks, shoulders, and overlapping reflections, and it often improves peak detection in patterns with sloped backgrounds or minor phases. Because derivative operations amplify noise, this method typically works best when appropriate preprocessing/smoothing and realistic thresholds are applied; otherwise it can produce false peak picks in noisy data.

σ cut

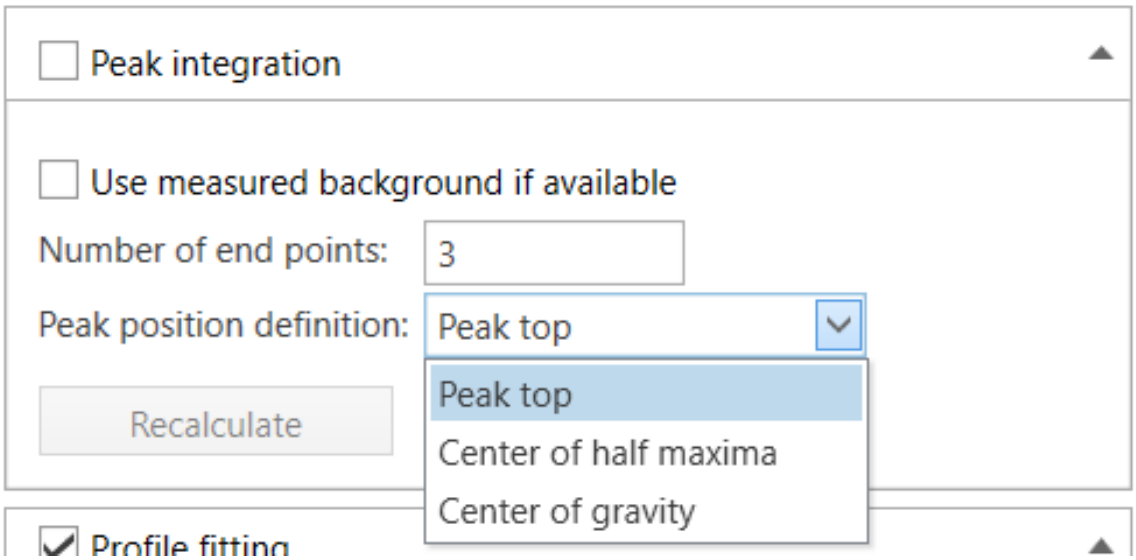
σ-cut (sigma cut) is a peak-detection threshold that tells the software how far a signal must rise above the local background/noise to be accepted as a real peak. Here, σ is the standard deviation of the noise (estimated from background regions), and the software typically accepts a peak only if its height is greater than (background + multiplier × σ). A setting of 3 means 3σ, i.e., the peak must be at least three times the noise level above the background to be counted as a peak.

Find amorphous peak

Find amorphous peak is an option that helps the software detect and report the broad diffuse "halo" in an XRD pattern that comes from amorphous or poorly crystalline material (e.g., glassy phases, polymers, disordered oxides), rather than sharp Bragg peaks from crystals. When enabled, the program looks for a wide hump-shaped maximum (often spanning several degrees in 2θ) and estimates its position, width, and intensity/area, which helps confirm an amorphous component and supports semi-quantitative comparisons between samples. Practical indicator: an amorphous halo is typically reported with a much larger FWHM than crystalline peaks, because the diffuse scattering is inherently broad. Use this option when a clear broad hump is present; avoid relying on it if the background fit is poor or fluorescence is high, since incorrect background handling can make the halo appear artificially stronger or weaker.

Peak integration

Calculates peak areas/strengths after defining background and peak boundaries. For qualitative ID it is optional but can help when comparing relative peak strength (e.g., major vs minor phase indications) and profile/Rietveld workflows when intensities are used.



Use measured background if available

Uses a measured/background dataset (if present) instead of estimating background mathematically. Helpful when fluorescence or high background makes peak detection difficult gives cleaner peak evaluation.

Number of end points

Number of end points controls how many data points on each side of a peak are used to define the start and end (integration limits) and to anchor the local baseline for area calculation. Using more end points can stabilize the baseline estimate (useful in noisy data), while too many can accidentally include neighboring peaks or peak tails; using too few can make the baseline sensitive to noise. A moderate value (e.g., 3) is often a practical starting point.

Peak position definition (Peak top)

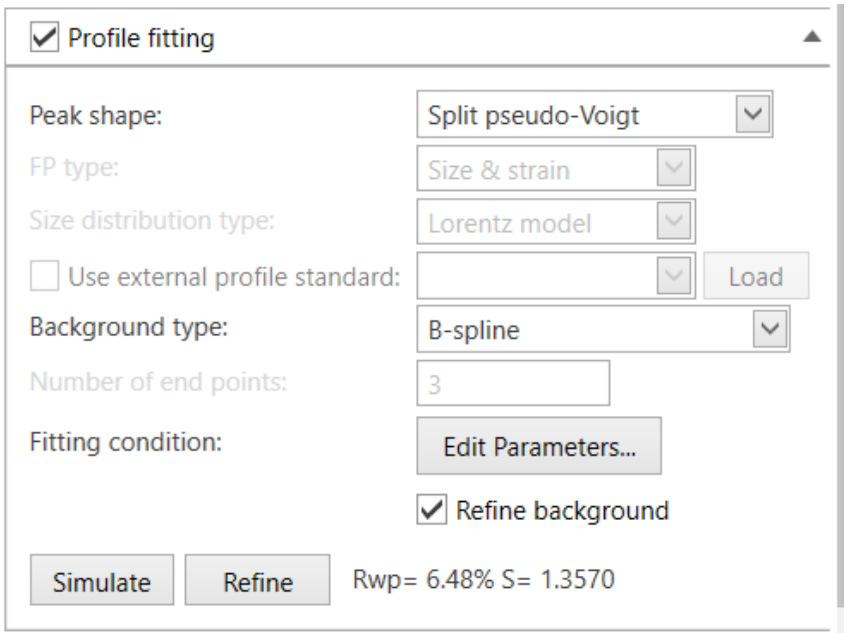
Peak position definition determines how SmartLab reports the peak 2θ position from the integrated profile. Peak top uses the maximum intensity point (fast and intuitive for sharp, isolated peaks). Center of half maxima reports the center at half height (often more stable than peak top when the peak is slightly asymmetric). Center of gravity uses an intensity-weighted centroid across the peak region (helpful for broad or asymmetric peaks and partially overlapped features, but more sensitive to correct background and integration limits).

Recalculate

Recalculate updates the peak integration results immediately using the current settings (background choice, end points, and peak position definition). Use it whenever you change any parameter so the peak positions and integrated areas in the Peak List reflect the new integration rules.

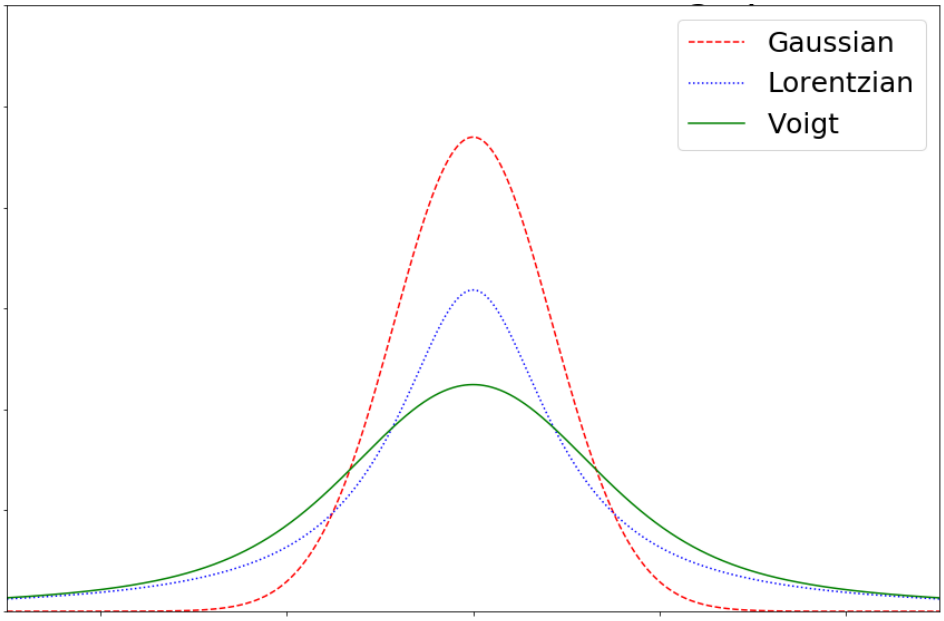
Profile fitting

Profile fitting models each diffraction peak using a mathematical peak-shape function plus a background, then adjusts the model parameters so the calculated pattern matches the measured data. It is used to obtain more reliable peak parameters (position, intensity/area, width/FWHM) and to handle overlap better than simple peak picking.



Peak shape (Split pseudo-Voigt)

Chooses the peak model used in fitting; pseudo-Voigt is widely used because real XRD peaks are mixed Gaussian/Lorentzian. Select Split pseudo-Voigt, Split Pearson VII, CALSA, FP method, Symmetric pseudo-Voigt, or Symmetric Pearson VII as the peak profile function used for profile fitting.



selection guide

- Peak looks symmetric → start with Symmetric pseudo-Voigt.
- Symmetric peak but tails need more flexibility → try Symmetric Pearson VII.
- Left and right sides are not equal → use Split pseudo-Voigt or Split Pearson VII.
- You want a physically based instrument/sample profile → use FP method.
- Data measured with CALSA high-resolution optics → use CALSA.

Background type (B-spline)

Defines how the background is modeled during fitting; B-splines give a smooth, flexible baseline. Good for qualitative work because it follows broad background trends without forcing the peaks to fit the baseline. Select one of the following: B-spline/Polynomial/Inverse polynomial/Line connecting endpoints.

Fitting condition (Edit Parameters...)

Fitting condition (via Edit Parameters...) controls what the software is allowed to refine and the limits/constraints during the fit (e.g., which peak parameters are fixed or free, ranges, tolerances, and any constraints). Use it to prevent unstable fitting, especially when peaks overlap or the signal-to-noise ratio is low.

Number of end points

Sets how many data points on the left and right sides of a peak region are used as the end/baseline anchors for background and profile fitting. Using more end points usually makes the baseline estimate more stable, but if too many points are included they may capture

neighboring peaks or a sloping background and distort the fit. For qualitative work, choose enough points to represent the local baseline clearly while staying outside adjacent peaks.

Refine background

Allows the background curve to adjust during fitting. When the Refine background box is selected, both peak profiles and background will be refined. When the Refine background box is cleared, only peak profiles will be refined but the background is kept fixed so your existing/edited baseline is preserved and not altered by the fitting routine.

Simulate

Simulate calculates and displays the pattern using the current model settings without performing an optimization. Use it as a quick preview to see whether the chosen peak shape and background type are reasonable before running a full refinement.

Refine

Refine runs the optimization step that iteratively adjusts the selected parameters (peak shape parameters, peak position/intensity/width, and optionally background) to minimize the difference between measured and calculated profiles. After refinement, review the fit quality numbers (Rwp, S) and visually check that the model follows peak shapes and valleys realistically.

Rwp, S

Rwp (weighted profile R-factor) and S (goodness-of-fit) are quick indicators of how well the calculated profile matches the measured XRD pattern: lower values generally mean a better fit. Rwp is reported as a percentage (lower is better; as a rough guide <5% excellent, 5–10% good, 10–15% acceptable, >15–20% poor), while S compares the remaining misfit to the expected statistical noise (ideal ≈ 1; 1–1.5 good, 1.5–2.5 fair, >3 poor). Use these numbers mainly as a sanity check for phase ID and peak evaluation, correct peak positions and realistic peak shapes/background matter more than chasing perfect Rwp/S values.

Automatic Phase Identification by Search/Match

Automatic Phase Identification (Search/Match) in SmartLab Studio II performs a database search/match by comparing the measured peak positions and intensities (generated in Peak Evaluation) against reference patterns from the installed PDF/ICDD (d-I) or other databases, then returns a ranked list of candidate phases. The function is best applied after the peak list has been cleaned (real peaks retained and artifacts/false picks removed), because the reliability of the suggested matches depends strongly on the quality of the input peaks; in routine workflows it serves as the primary tool for rapid qualitative phase identification. The output populates the Search results / Candidate phase lists and typically supports overlaying reference peak markers/patterns on the measured scan so agreements and mismatches are immediately visible.

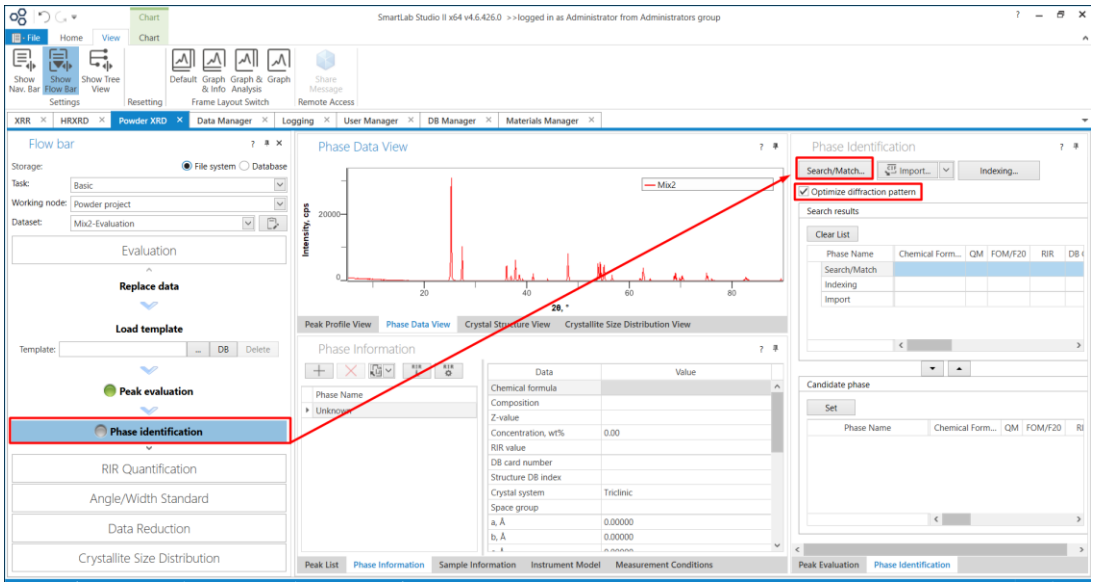
Load file → perform peak evaluation → Click Phase identification → Search/Match (confirm Optimize diffraction pattern checkbox is selected).

Optimize diffraction pattern

Optimize diffraction pattern improves Search/Match reliability by applying internal optimization during phase identification: when the box is ticked, SmartLab Studio II conditions the pattern for matching (e.g., improved baseline handling/smoothing) and may also optimize the selected reference card (lattice parameters) to better align calculated peak positions with the measured pattern before listing it in the results, which typically gives cleaner, more stable candidate rankings. When the box is cleared, reference cards are compared and added as-is and the matching uses the pattern without this extra optimization, which can preserve subtle real features but may increase false/less-stable candidates if the data are noisy or the baseline is imperfect.

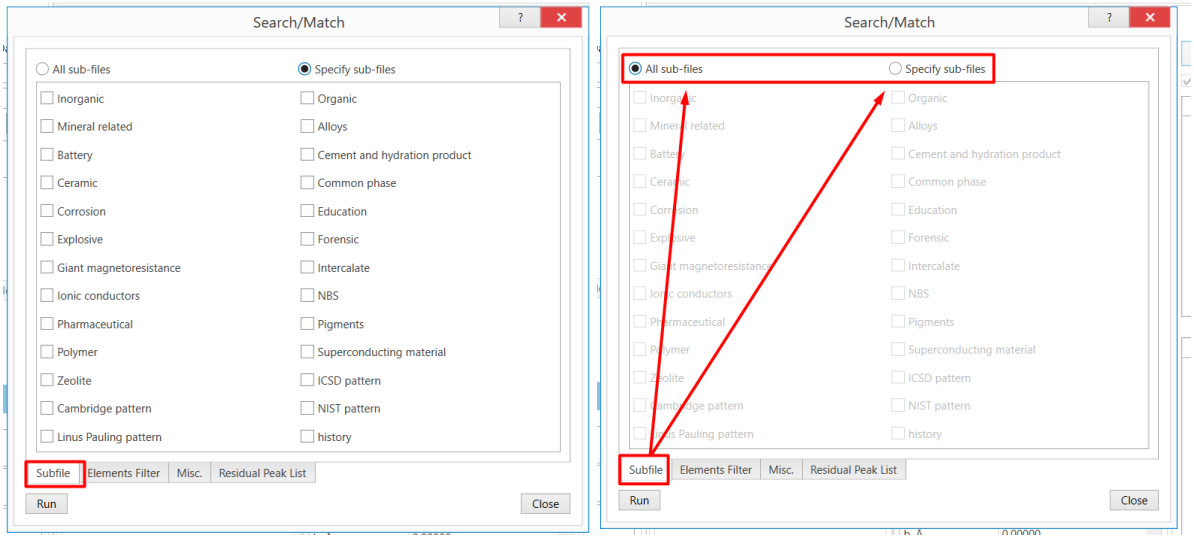
Ticked = cleaned measured pattern + better-aligned reference card for more reliable Search/Match.

Unticked = more direct/raw comparison.



Subfile

When using the ICDD PDF-2 database, the Subfile option filters the classes of materials that will be searched during Search/Match. This narrows the search space, reduces false matches, and increases the chance that the expected phase appears near the top of the candidate list. Subfiles should be selected based on sample type and origin (e.g., mineral, ceramic, alloy, battery, polymer) and any known processing/environment (e.g., corrosion products, cement hydration). If the sample is unknown, it is better to start broad (e.g., Inorganic / Common phase) and then narrow the subfiles after an initial result. Select only the checkboxes that realistically match the sample to keep the candidate list accurate and manageable.



Elements filter

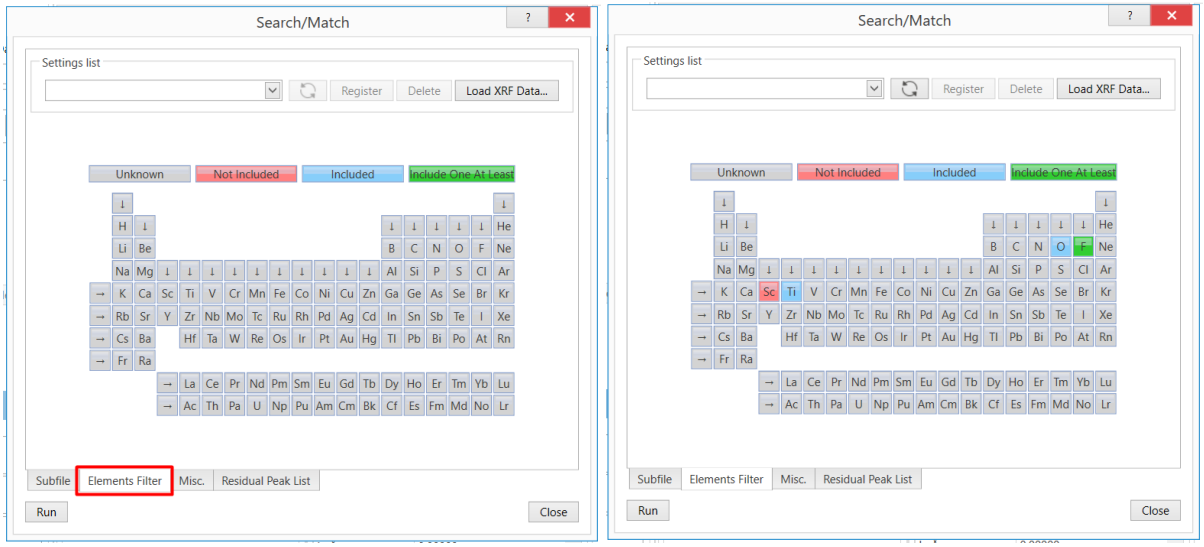
The Elements filter is used to restrict Search/Match to only those PDF-2 entries whose chemical composition is consistent with the sample. By excluding impossible phases and prioritizing chemically realistic ones, it significantly improves the ranking and reliability of the candidate list especially when peak overlap or high background makes pattern-only matching uncertain. Each element can be assigned one of four states (colors), which act as chemical rules during the search:

- **Grey – Unknown:** No condition is applied; the element is ignored in filtering.
- **Red – Not Included**: Candidate phases must not contain this element (useful to eliminate obvious false matches).
- **Blue – Included:** Candidate phases must contain this element (use when an element is confirmed to be present and diagnostic).
- **Green – Include at Least One:** Candidate phases must contain at least one of the green-marked elements (useful for mixtures where different phases may contain different key elements).

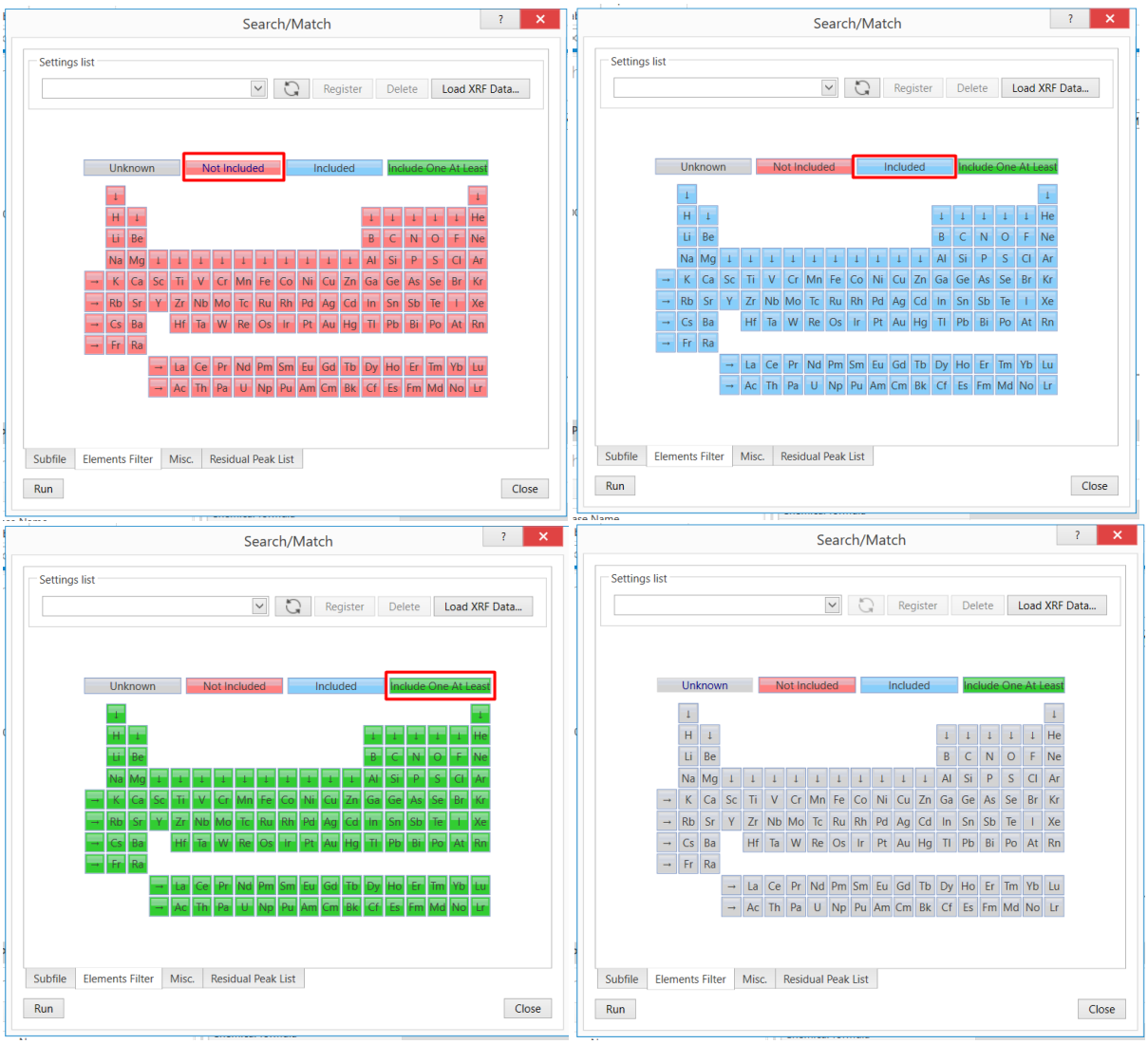
Conditions can be set manually by clicking an element to cycle through: Unknown → Not Included → Included → Include at least one. In practice, Blue should be used only for elements that are confidently present (e.g., from synthesis recipe or XRF/EDS), because forcing an element can unintentionally remove the correct phase if the element is only present in trace form or in an amorphous component. “Green (Include at least one)” is used when the sample may contain different phases with different compositions, so it is risky to force one single element to be present in *every* candidate. Example: if a mixed sample could contain TiO_2 (Ti), Al_2O_3 (Al), and an iron oxide (Fe), marking Ti, Al, Fe as green tells the software: *“Return phases that contain at least one of these elements.”* This keeps all realistic phase families in the search, but still filters out unrelated phases that contain none of those key elements—so the search is narrowed without being too strict.

For best results, keep the filter chemically realistic but not overly strict: use Red to exclude elements that are truly impossible (e.g., Cl-free processing, no heavy metals), use Blue for

confirmed major elements, and use Green when multiple phase families are expected. The filter can also be populated efficiently using Load XRF Data...; importing XRF results lets the software automatically assign element states based on measured composition, providing a strong starting point that can then be fine-tuned for qualitative phase identification. The green setting is recommended when analysing complex mixtures, where different phases may contain different sets of elements.

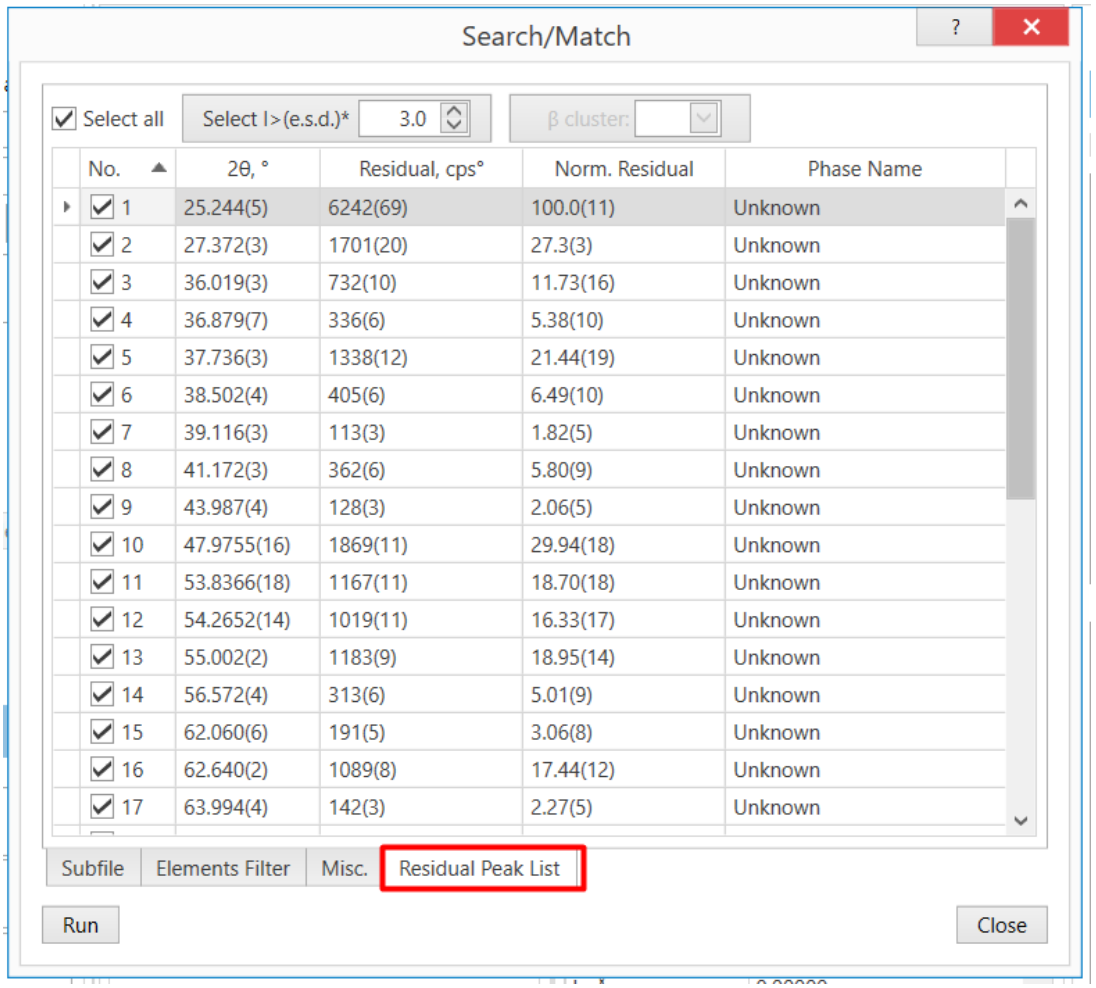


It is also possible to select search conditions collectively in this way.

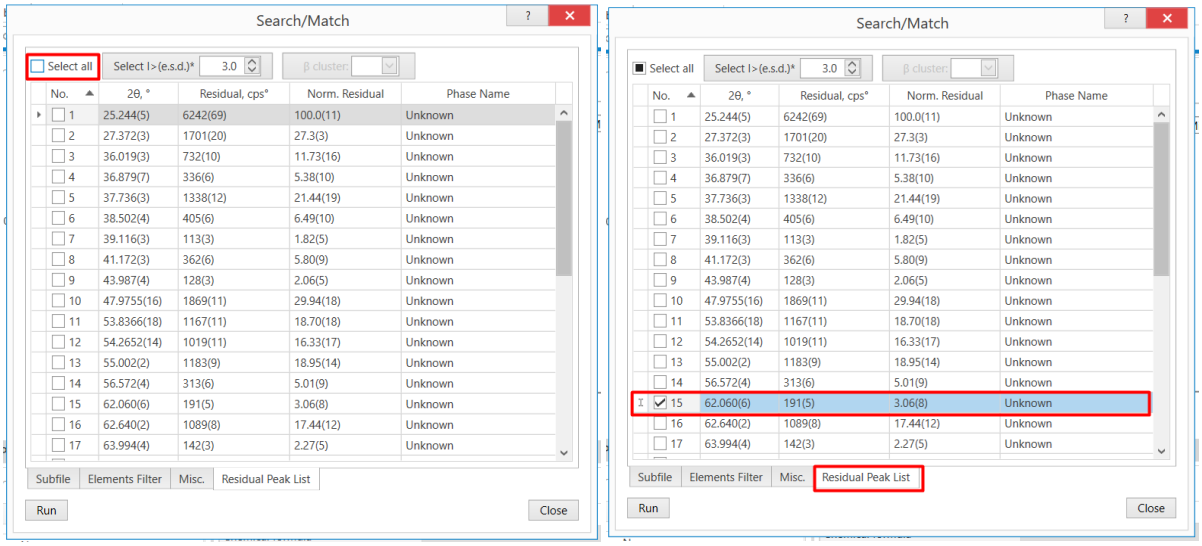


Residual Peak List

The Residual Peak List allows Search/Match to be performed using only the peaks selected in this list. For example, if a weak peak remains unexplained after identifying the main phase(s), that peak can be selected alone so the software searches specifically for phases that could account for it. This is particularly helpful for finding minor, impurity, or overlapping phases that are masked in the full pattern search. It is best used as a follow-up tool after the primary identification step, while the Elements Filter remains the most commonly used option for routine, chemistry-guided phase searching.



For instance, when a small peak remains unassigned, deselect *Select All* and select only the checkbox for the unidentified peak to perform a search focused on that peak.



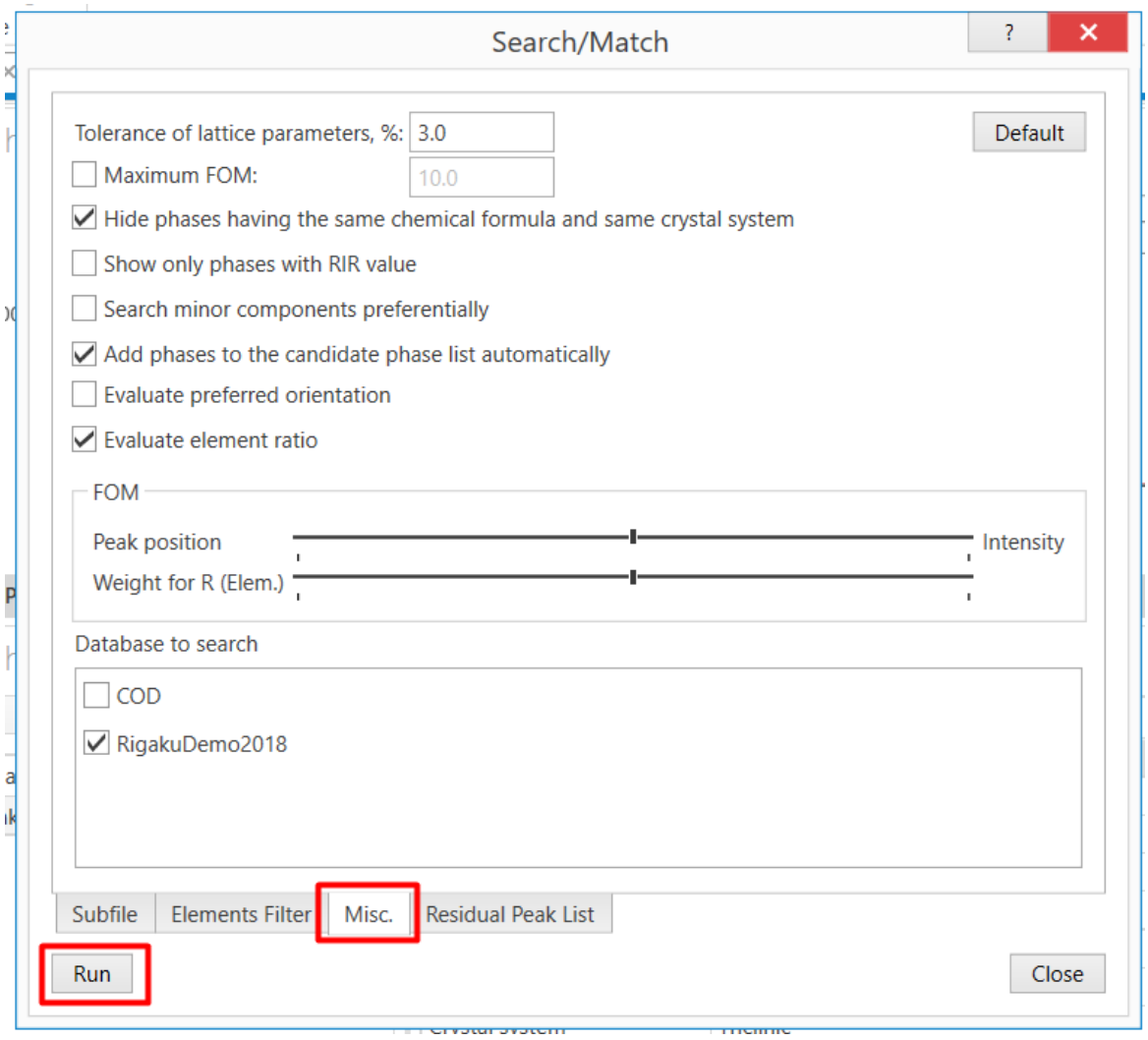
Miscellaneous

The Misc. tab contains advanced Search/Match controls that fine-tune how candidates are ranked and filtered, helping produce cleaner and more meaningful phase-ID results. For routine

qualitative identification, these options are mainly used to reduce duplicate hits, control matching strictness, and bias the search toward phases that better explain the measured pattern.

Key settings and their practical use include: Tolerance of lattice parameters (%), which defines how far the reference lattice parameters may be adjusted/accepted during matching (useful for solid solutions or slight strain); and options such as Hide phases having the same chemical formula and same crystal system, which suppresses near-duplicate entries so the results list is easier to interpret. If quantitative methods like RIR are intended, Show only phases with RIR value restricts the result list to entries that include RIR information; otherwise, leave it unchecked to avoid unnecessarily removing valid qualitative candidates. Additional checkboxes (e.g., Search minor components preferentially, Evaluate preferred orientation, Evaluate element ratio) can help highlight minor phases, handle texture effects, or enforce chemical plausibility these are most useful when the sample chemistry is known (from recipe, XRF/EDS). The Database to search section allows selecting one or more available databases (e.g., installed Rigaku/CIF-based databases), and Default restores the software's recommended baseline settings for this tab.

When required settings are completed, then click RUN button.



Search results is the complete, ranked output of Search/Match i.e., all database phases that show a possible match to the measured pattern based mainly on peak positions (and, depending on settings, relative intensities and lattice-parameter optimization). It is a "suggestion list" that may include correct phases as well as chemically unrealistic or duplicate hits.

Candidate phase is the smaller, user-confirmed set selected from the Search results (or chosen automatically by the software) that represents the most likely phases actually present. Only candidates are treated as "active" phases for practical checking such as overlaying reference peak bars/patterns, assigning peaks in the peak list, and building a consistent multi-phase interpretation by explaining the remaining unidentified peaks.

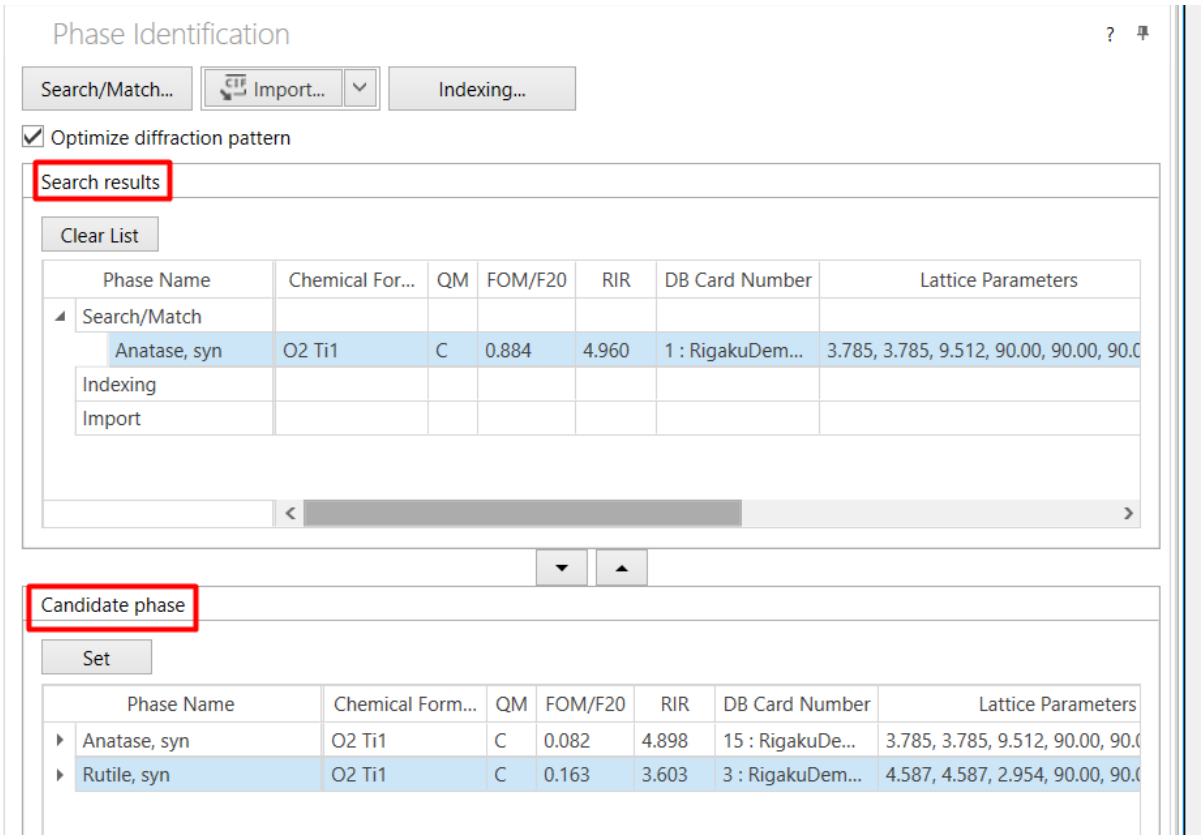


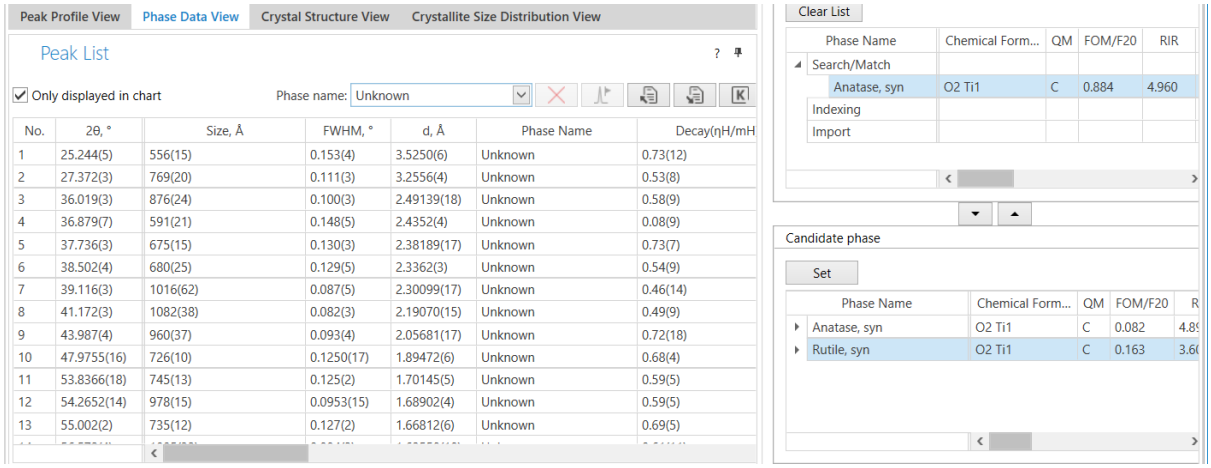
Figure of Merit (FOM)

Figure of Merit (FOM) is a match-quality index used by SmartLab Studio II to rank Search/Match results according to how well a database reference pattern agrees with the measured XRD data. In general, a lower FOM indicates a better match, meaning the candidate's peak positions (and, depending on settings, intensities) align more closely with the measured peaks and fewer strong peaks remain unexplained. FOM is therefore a useful first guide for selecting likely phases; however, final selection should still be confirmed by checking the peak-bar overlay for missing strong predicted peaks, unexplained measured peaks, and chemical plausibility. In the example shown, the phase with the smaller FOM would be considered the more reliable match than a phase with a larger FOM.

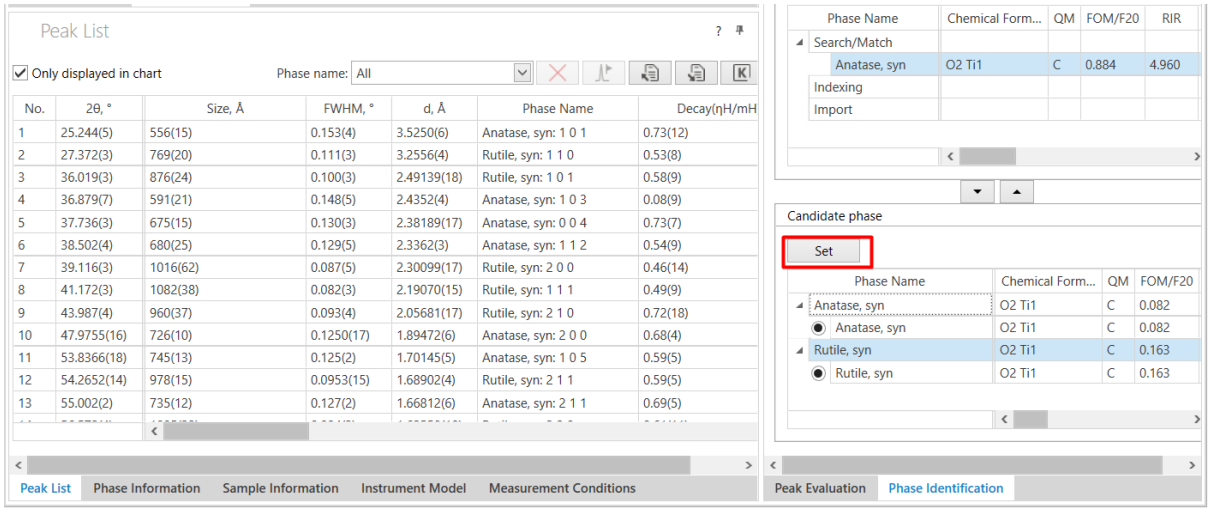
Phase Names in Peak List

After suitable phases have been selected and confirmed, SmartLab Studio II assigns those phases to matching peaks, and the corresponding phase name (and related indexing information, where available) appears in the Phase Name column of the Peak List. Peaks that remain labeled “Unknown” indicate reflections that are not explained by the currently selected candidate phase(s). In this situation, the phase search should be repeated typically by running Search/Match again and, if needed, using a targeted search on the unexplained peak(s) (Residual Peak List) to identify possible minor/impurity phases.

Before assuming “Unknown” peaks represent a new phase, it is important to verify peak quality. Poor peak evaluation can leave noise peaks, Kβ-related features, or background artifacts in the peak list, and these will often remain unassigned. Therefore, each “Unknown” peak should be checked against the raw profile (shape, intensity, repeatability) and the instrument/source conditions to confirm whether it is a true diffraction peak or an artifact (noise/Kβ), and only then should it be used to drive additional phase searching.

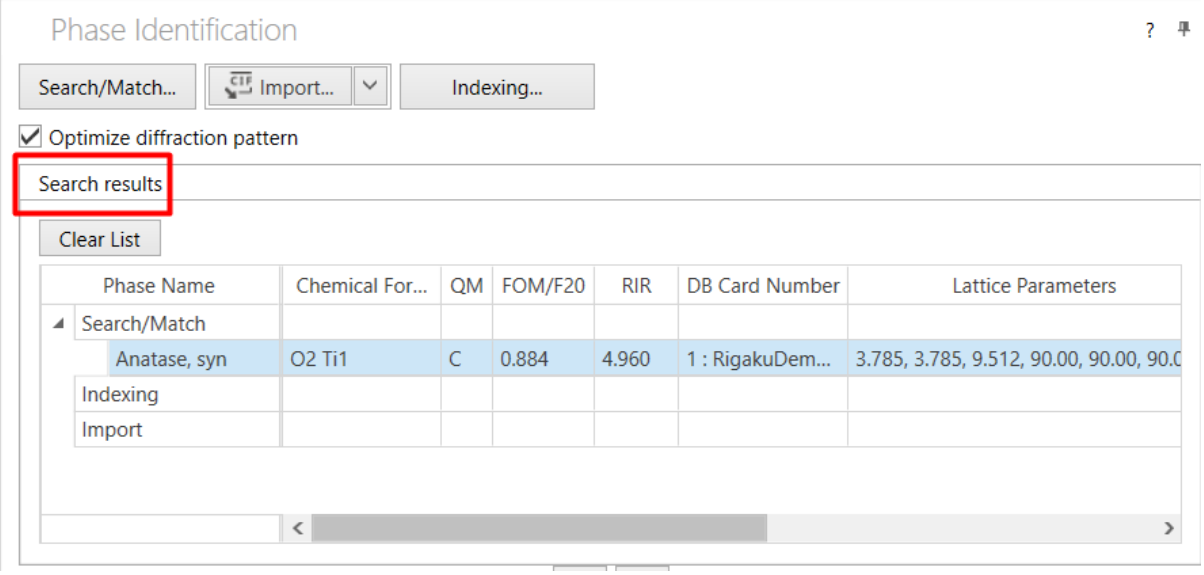


If the candidate phase list is final then press Set



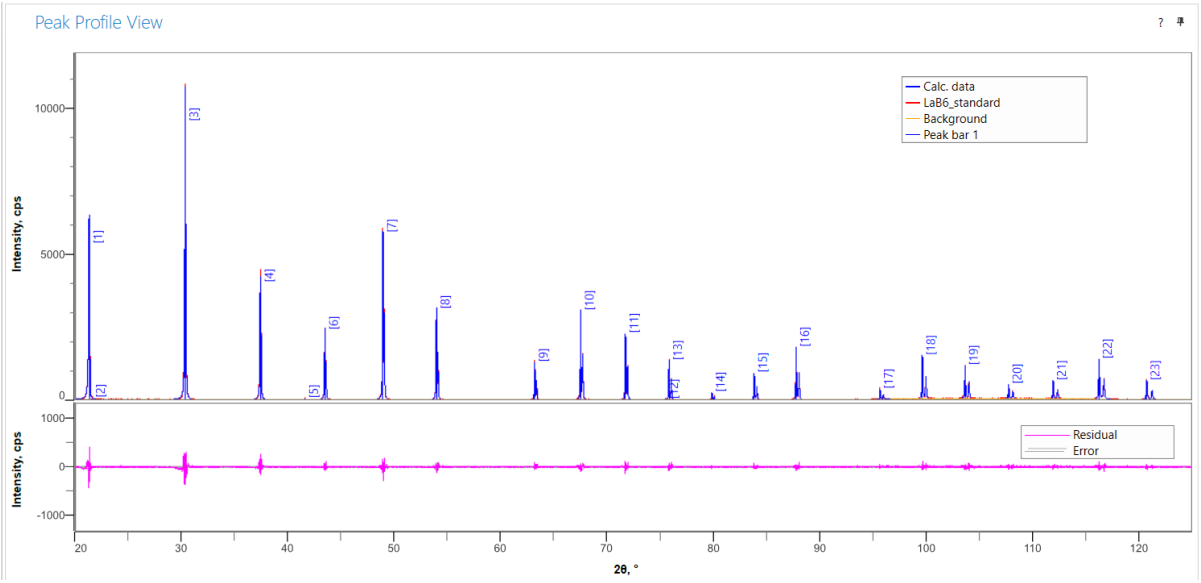
Only displayed in chart filters the Peak List to show only the peaks that are currently visible in the plotted 2θ range. Check it when working on a specific region (zoomed view) to quickly

edit/verify peaks without scrolling through the full list. Its effect is display-only: it does not change the data or peak fitting just hides peaks outside the current chart window.



Residual is the point-by-point difference between the measured XRD intensity and the calculated/fitted intensity, while the Error trace shows the expected statistical uncertainty of the measured counts from counting statistics.

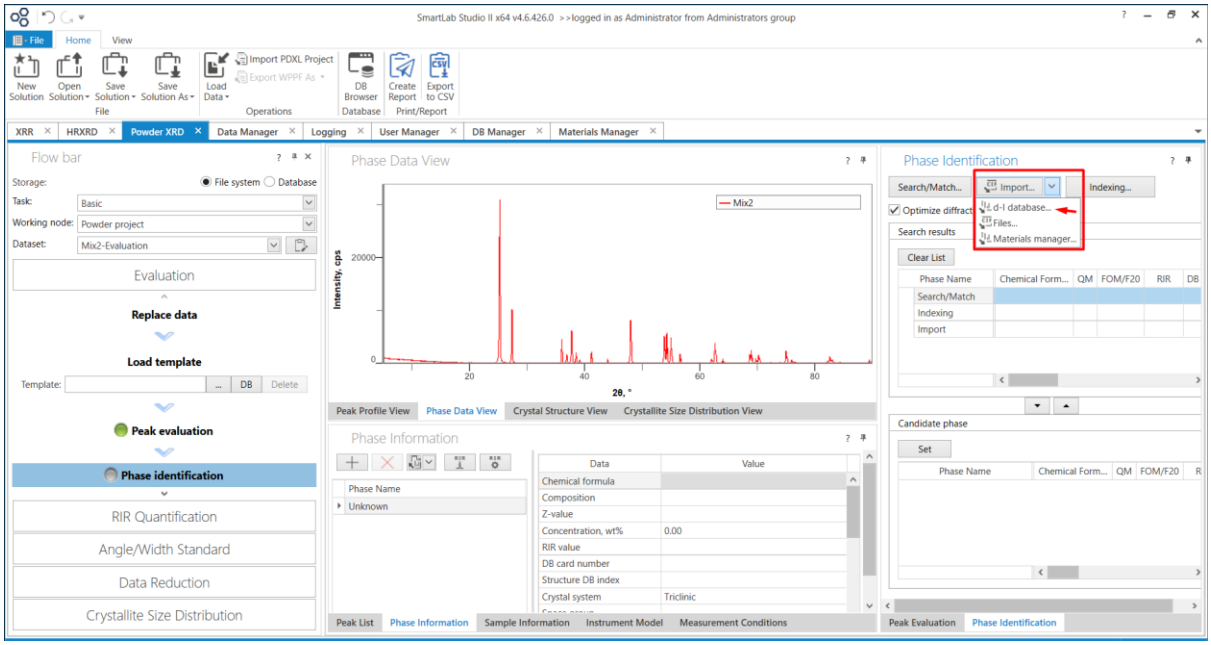
A fit is considered good when the residual fluctuates randomly around zero and stays mostly within the error trace; large or systematic deviations suggest that the model does not fully describe the data, often due to incorrect peak position, intensity, width, background, or phase/model choice.



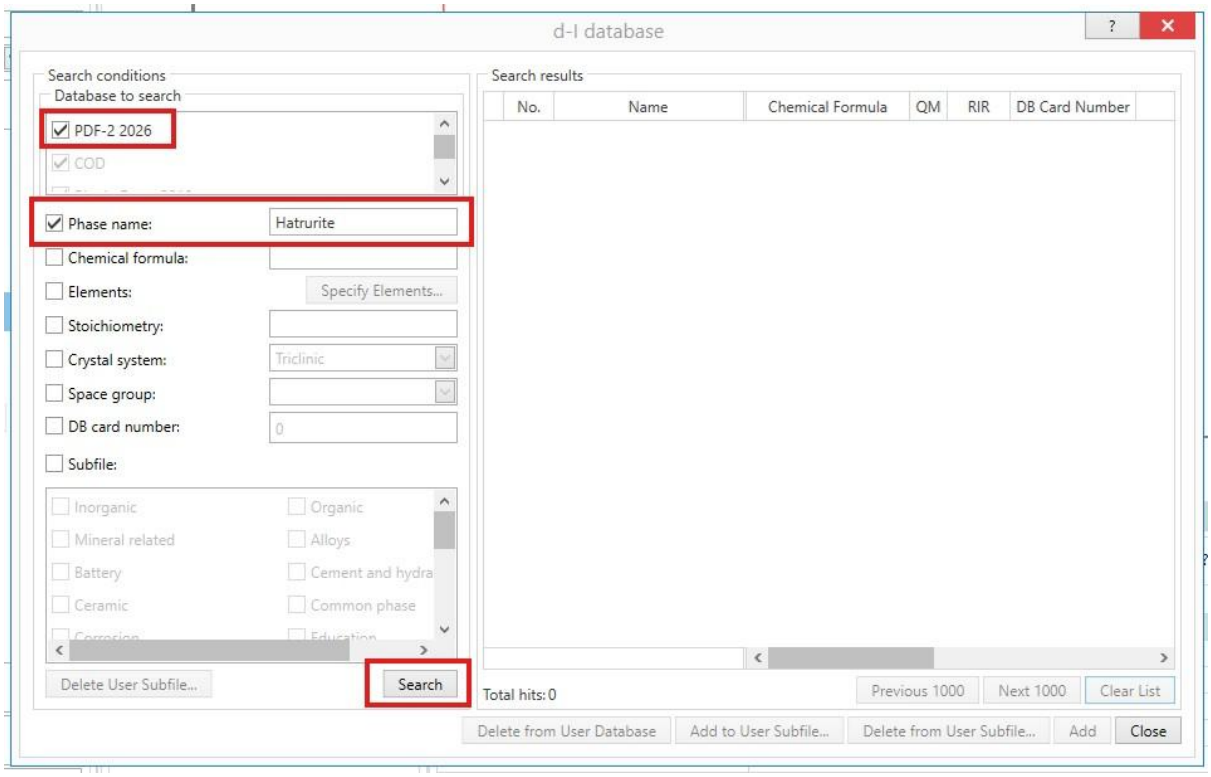
Phase Identification by d-I (PDF-2) Database Import

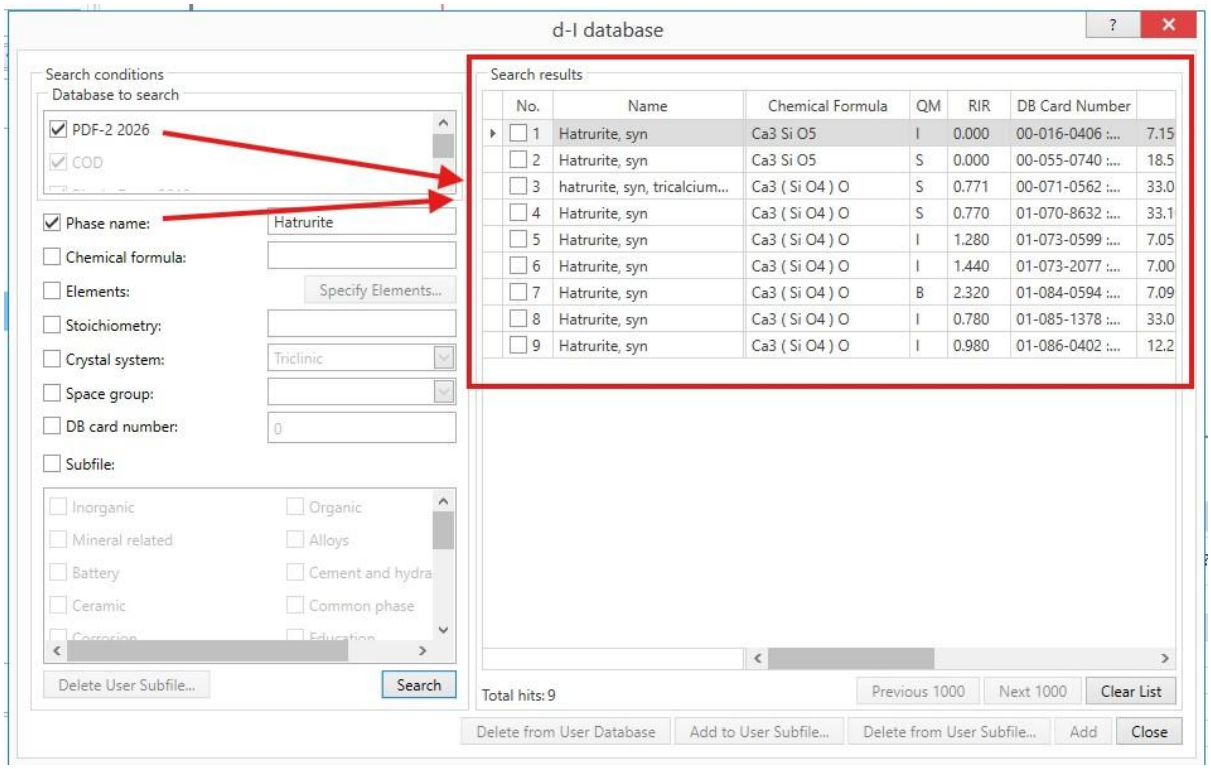
Manual phase identification using the d-I (PDF-2) database is performed by selecting the target database (e.g., PDF-2 2026) and then applying one or more search conditions for example a phase name such as *Hatrurite*. This approach is most valuable when the expected phase is already known (fully or partially), or when automatic Search/Match misses weak or minor peaks due to overlap, background, preferred orientation, or low intensity.

The d-I search allows targeted filtering using practical identifiers such as phase name, chemical formula, elements, stoichiometry, crystal system/space group, or a specific DB card number. After clicking Search, the matching cards are listed; the correct entry can then be verified and selected, and imported by ticking the checkbox and clicking Add. In practice, this method improves reliability by forcing the comparison against a known, chemically plausible phase, and it is especially effective as a confirmation tool—i.e., importing a suspected phase to overlay its peak positions and check whether it explains the unexplained reflections before expanding the candidate list further.

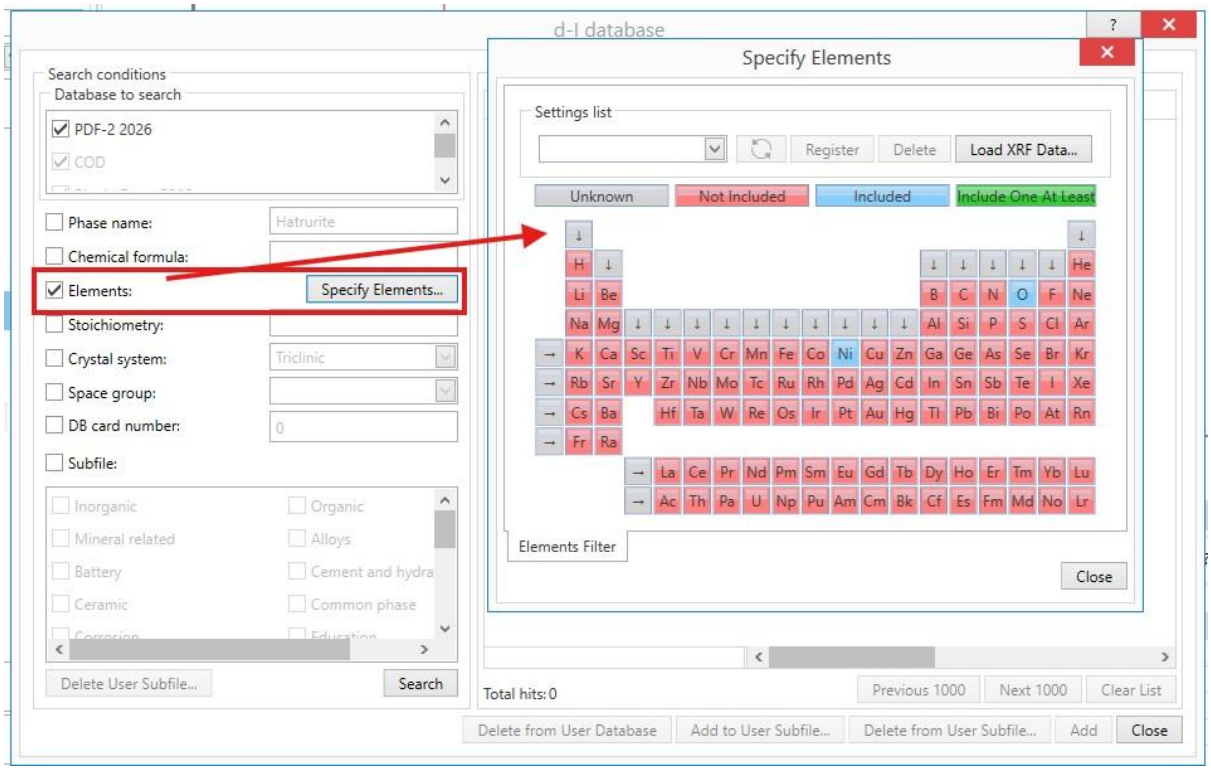


This example demonstrates entering the name of the crystalline phase in the *Phase Name* field and clicking *Search*, which displays the corresponding target crystal phase.

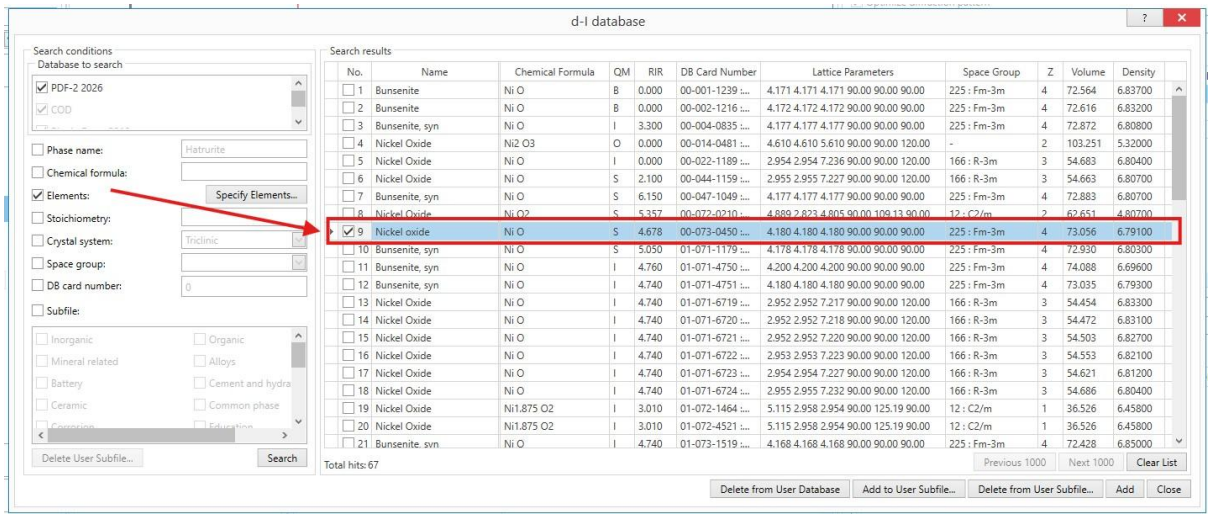




Similarly, entering the elemental information associated with the target crystalline phase in the *Elements* field and clicking *Search* displays the corresponding crystalline phase.



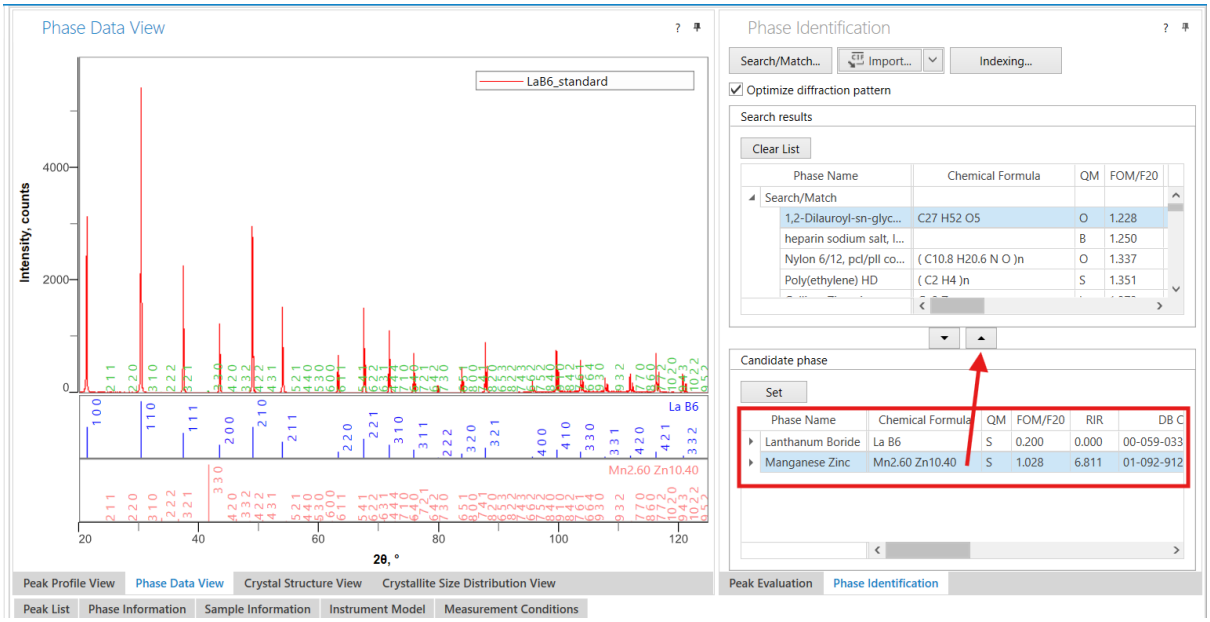
After locating the desired card, select its corresponding checkbox and click the *Add* button.



Worked Example: XRD Phase Identification and Reporting

The report contents should be selected based on purpose typically measurement conditions, the measured diffraction profile, and the final phase identification/phase information for a paper.

Analysis of the sample Lanthanum Hexaboride (LaB_6)



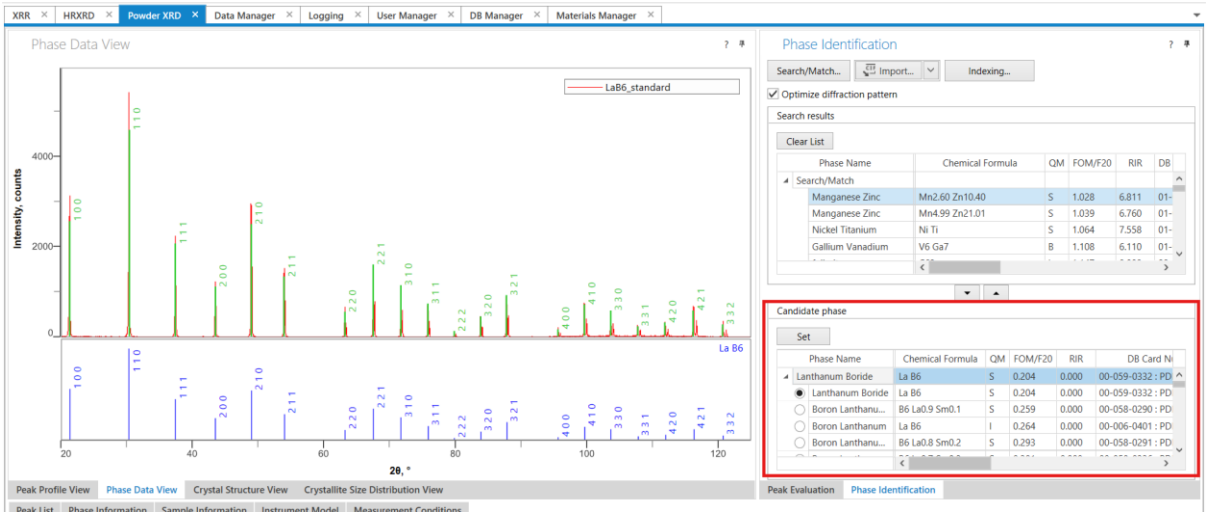
Phase Selection Rules (PDF-2 Search/Match)

From the screenshot, Lanthanum Boride (LaB_6) appears in the *Candidate phases* list along with an unlikely second phase (e.g., "Manganese Zinc …"), while the *Search results* list also contains clearly chemically irrelevant organic entries this is a common artifact of automated matching when peak lists include overlaps/noise or intensity weighting is high.

How to decide whether one phase or two are real (practical rules):

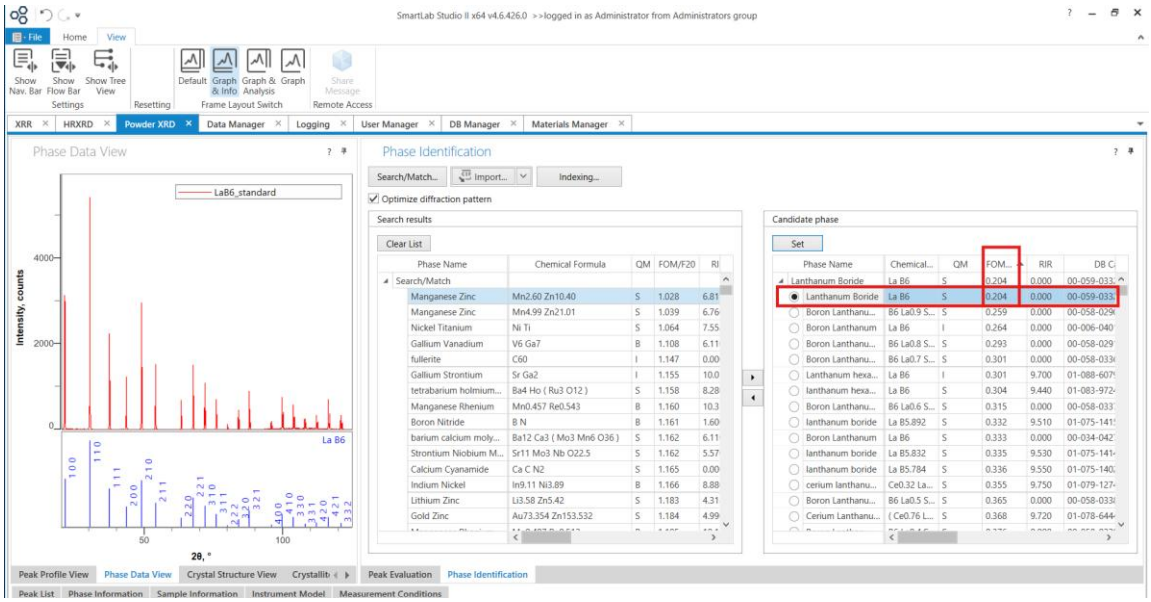
1. Chemistry first (hard filter): keep only phases consistent with known/expected elements (set Elements Filter to La + B for this training sample; also restrict to Inorganic subfiles). Anything like polymers/organics can be discarded immediately.
2. Coverage of peaks (strongest criterion): the main phase should explain all major measured peaks (positions) and most minor ones; accept a second phase only if it explains remaining unmatched peaks after the primary phase is applied.
3. "3-peak rule" for a minor phase: a secondary phase is credible only if ≥3 of its strong lines appear at the correct 2θ without relying on overlaps with the main phase.
4. Intensity sanity check: relative intensities should be *reasonable*; if the candidate's strongest line is absent or extremely weak while weaker lines "match," it is usually a false positive.
5. Residual peak list check: after selecting LaB_6, look at Residual Peak List if residuals are just noise/trace bumps and no consistent pattern remains, keep single-phase LaB_6.

Bottom line for this LaB_6 dataset: select LaB_6 as the primary (and likely only) phase, and treat the second candidate as spurious unless it uniquely accounts for several clear residual peaks with correct intensity behavior.

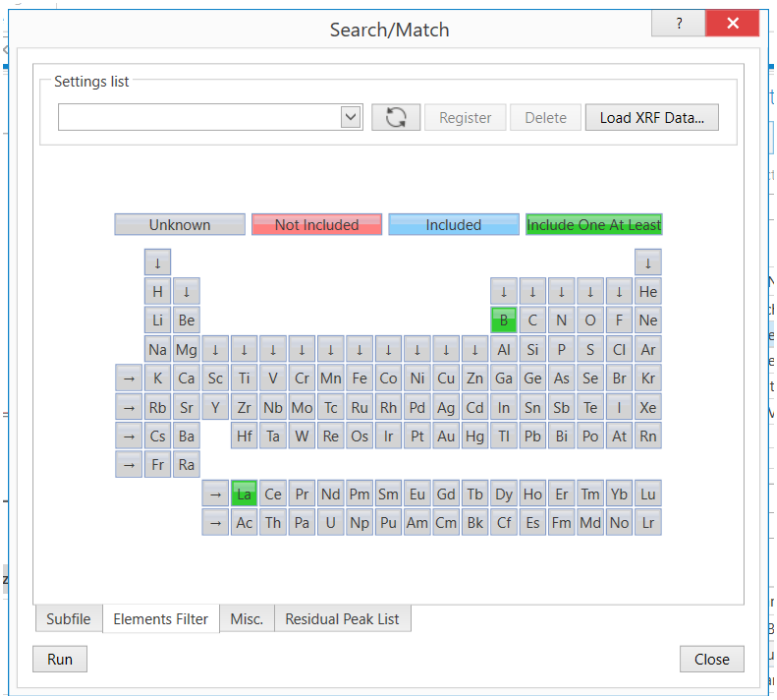


Selecting the Correct PDF-2 Candidate (when many "LaB_6 / Lanthanum Boride" entries appear)

1. Filter by chemistry first: keep only entries with exact formula LaB_6 (discard "Boron–Lanthanum …" variants unless the formula is identical).
2. Pick the best match statistic: sort candidates by FOM/F20 and start with the lowest value (best fit to peak positions/intensities).
3. Prefer highest data quality: choose entries with the best QM/quality mark (higher-quality evaluated/reference patterns) and with a valid RIR (helps later quantification).
4. Validate by overlay, not the number: select the candidate whose stick pattern explains all major peaks and leaves minimal residual peaks; accept a second LaB_6 entry only if it uniquely explains peaks the first one cannot (rare for a single-phase standard).
5. Use the most complete reference: prefer the card that contains indexed peaks + lattice parameters/space group (best for refinement and consistency checking later).

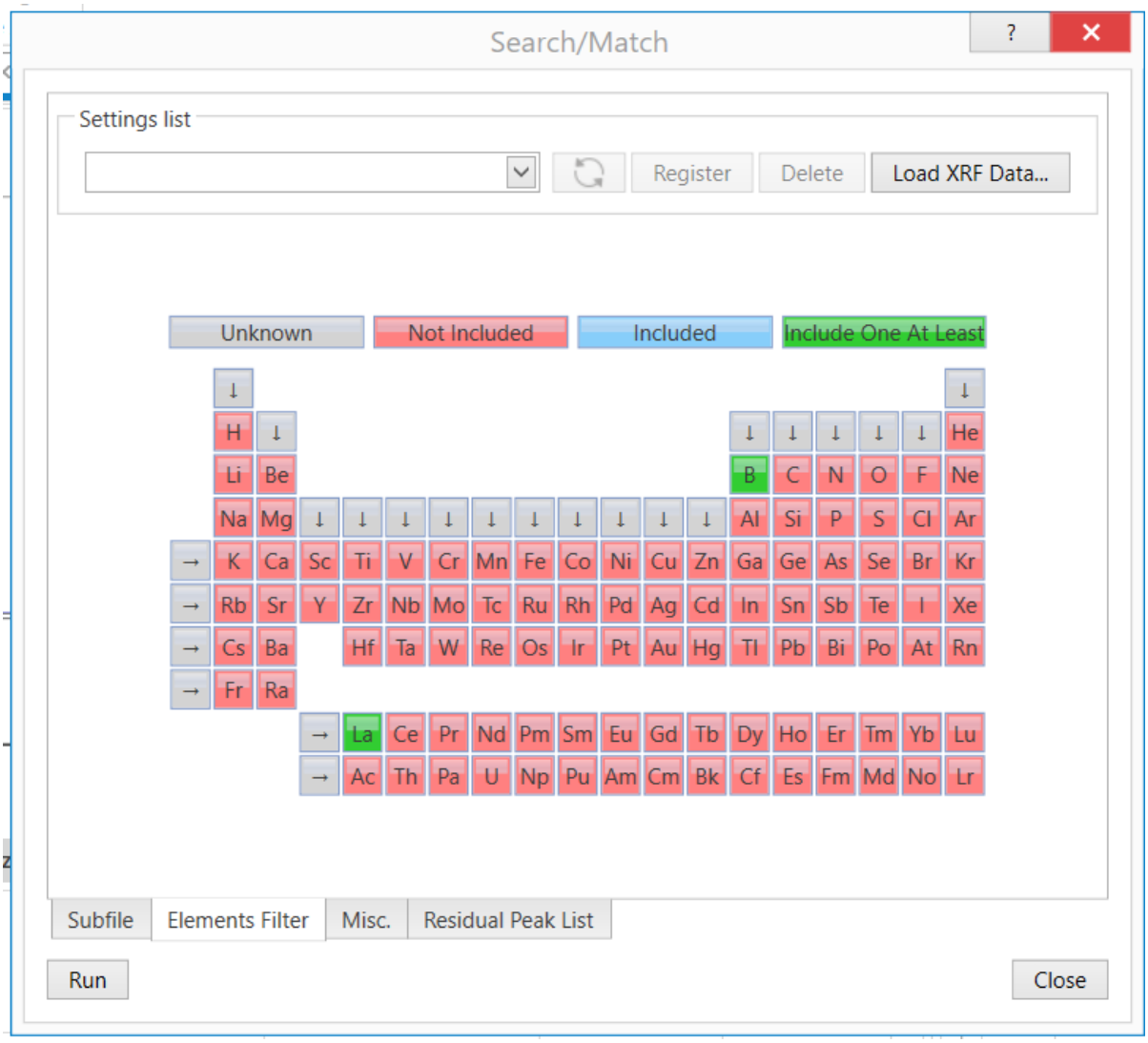


The selection is conceptually correct: the chosen Lanthanum Boride (LaB_6) entry sits at the lowest FOM/F20 (~0.204) and its stick pattern aligns with the dominant peak set, so it is the best primary candidate. Critically, the candidate list contains multiple LaB_6 cards with very similar FOM, so the most reliable choice is the one with higher QM (better evaluated data) and richer card metadata (indexed peaks/lattice parameters/RIR if later quantification is needed). The long "Search results" list above (Mn–Zn, Ni–Ti, polymers, etc.) indicates the search is still chemistry-underconstrained, so applying an Elements Filter (La+B) and restricting to inorganic/ceramic subfiles will reduce false positives and make minor-phase decisions depend mainly on residual peaks, not database noise.



Elements Filter Check (Known LaB_6 Sample)

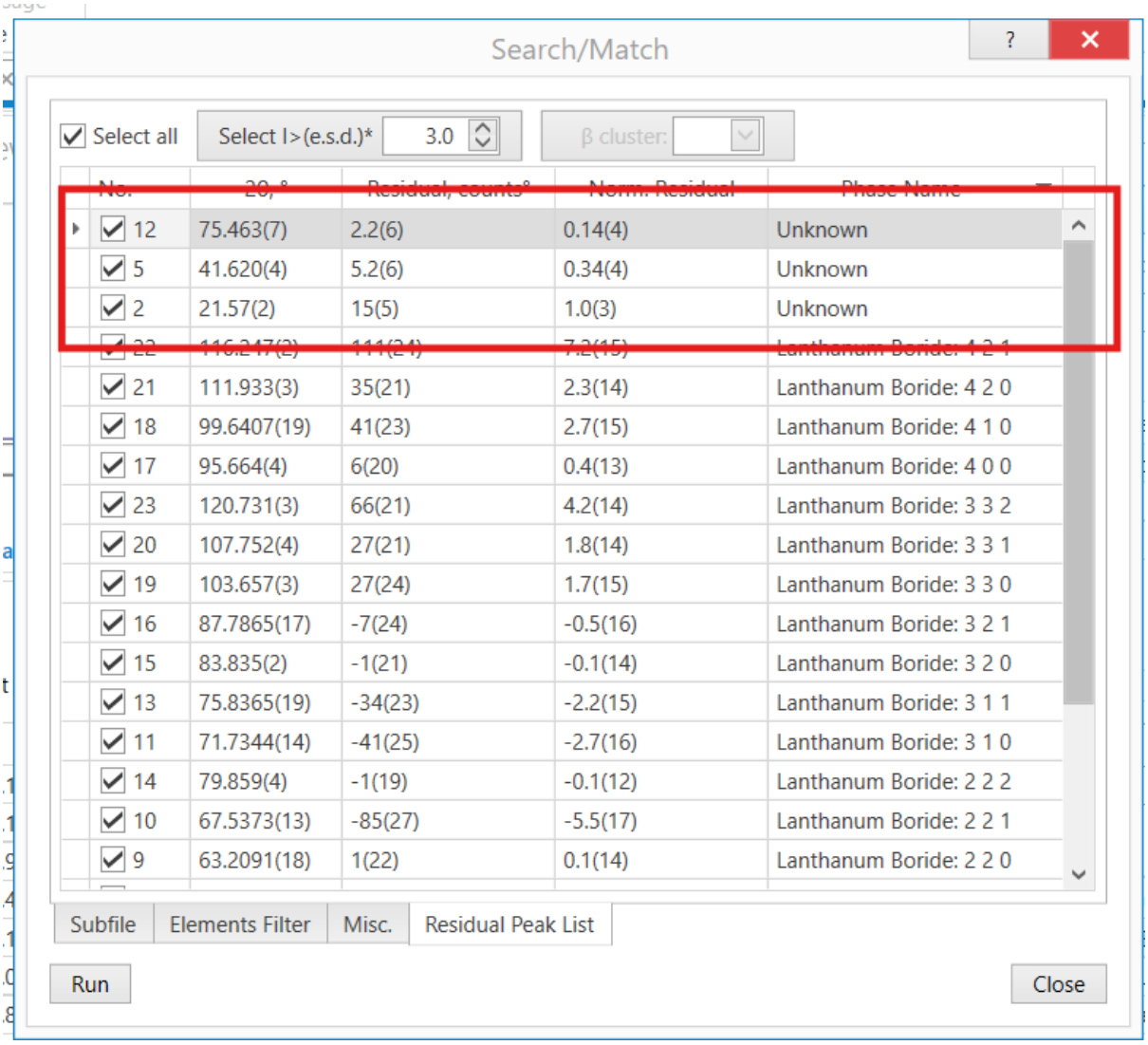
The Elements Filter configuration shows B and La marked as included (green), while most other elements remain unassigned (grey). This is an appropriate starting point for a known LaB_6 specimen, because the PDF-2 Search/Match is guided toward phases containing La and B, reducing chemically unrelated matches. For cleaner, more selective results, set La and B to "Include One At Least" (must contain) and set common organic false-positive elements (C, H, O, N) to "Not Included" when working with an inorganic ceramic; these restrictions should be relaxed only when screening for possible impurities or contamination.



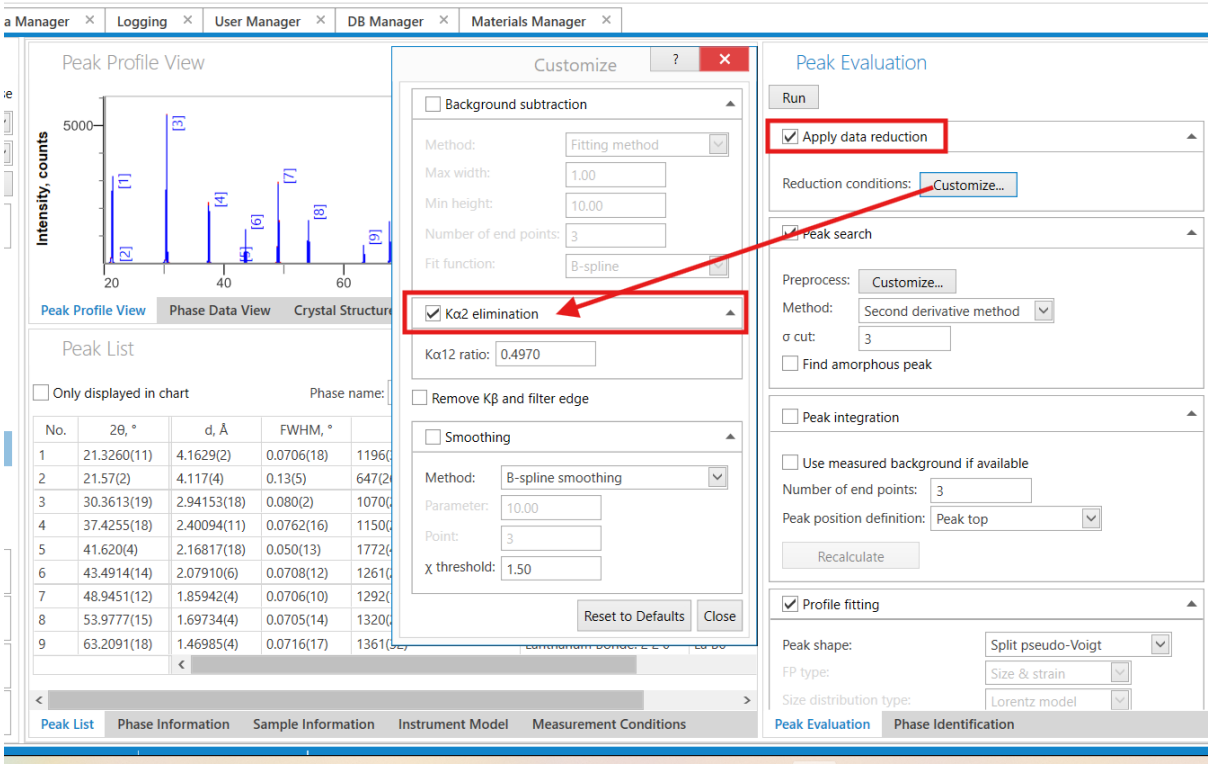
Elements Filter Setting (LaB_6 Confirmation vs. Impurity Screening)

In the Elements Filter, La and B are set to “Include One At Least” (green) while most other elements are set to “Not Included” (red). This configuration forces PDF-2 Search/Match to return phases containing La and/or B, making it well suited for confirming LaB_6 and suppressing chemically unrelated matches.

Caution: This setting is intentionally restrictive and can mask genuine secondary phases/contaminants (e.g., oxidation/hydration products or sample-holder/adhesive contributions). For impurity screening, keep La and B as required, but set likely impurity elements (commonly O, C, Si, Al) to “Unknown” rather than “Not Included” to allow plausible impurity candidates to appear.

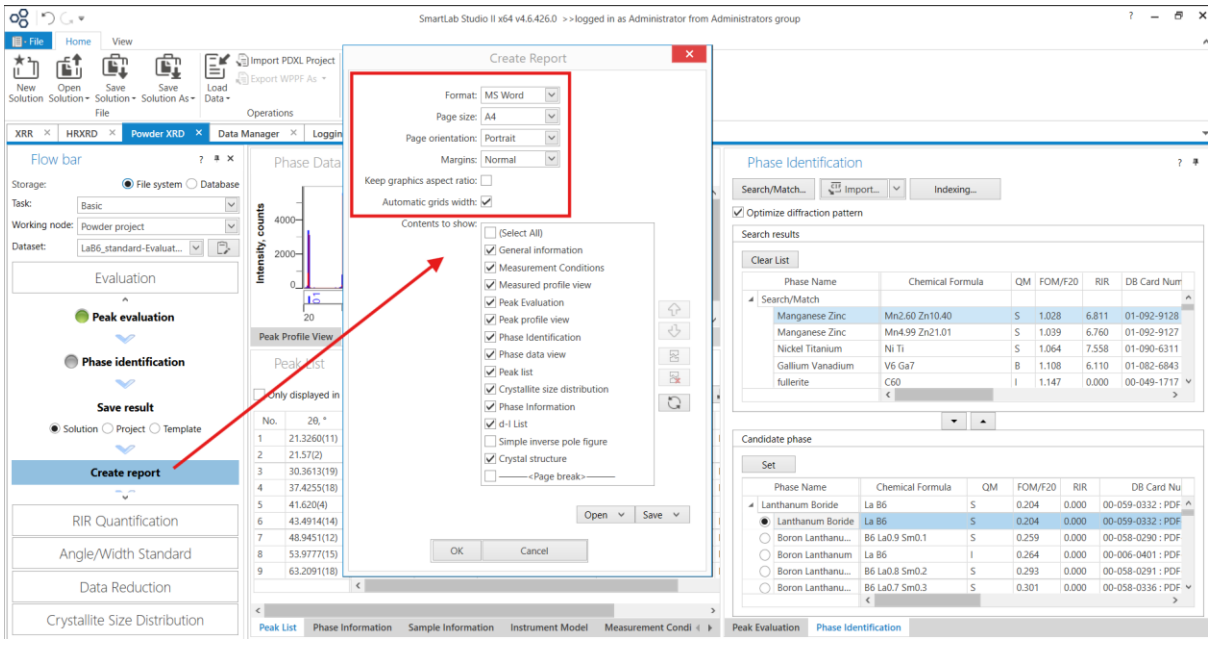


If the specimen is strictly single-phase LaB_6, those “Unknown” peaks should be treated as residual artifacts from background/low-angle scatter, sample displacement/zero-shift, or imperfect $K\alpha_2$ stripping/profile fitting not as real phases. A true impurity would typically generate multiple consistent lines; the next action is to refine background/zero shift and re-check the residual list rather than adding a second phase.



Quality Mark (QM) in PDF-2 is ICDD's reliability label for each database entry and indicates how trustworthy that reference card is for phase identification and interpretation. For practical analysis, prioritize **★ / R / I** entries first, and treat **B / O / C / H / P** entries with caution by checking editorial comments or filtering them out when necessary. [rigaku.com] [rigaku.com], [resources.rigaku.com]

Once the analysis is complete, the report will be prepared.



Report of the sample Lanthanum Boride (LaB_6)

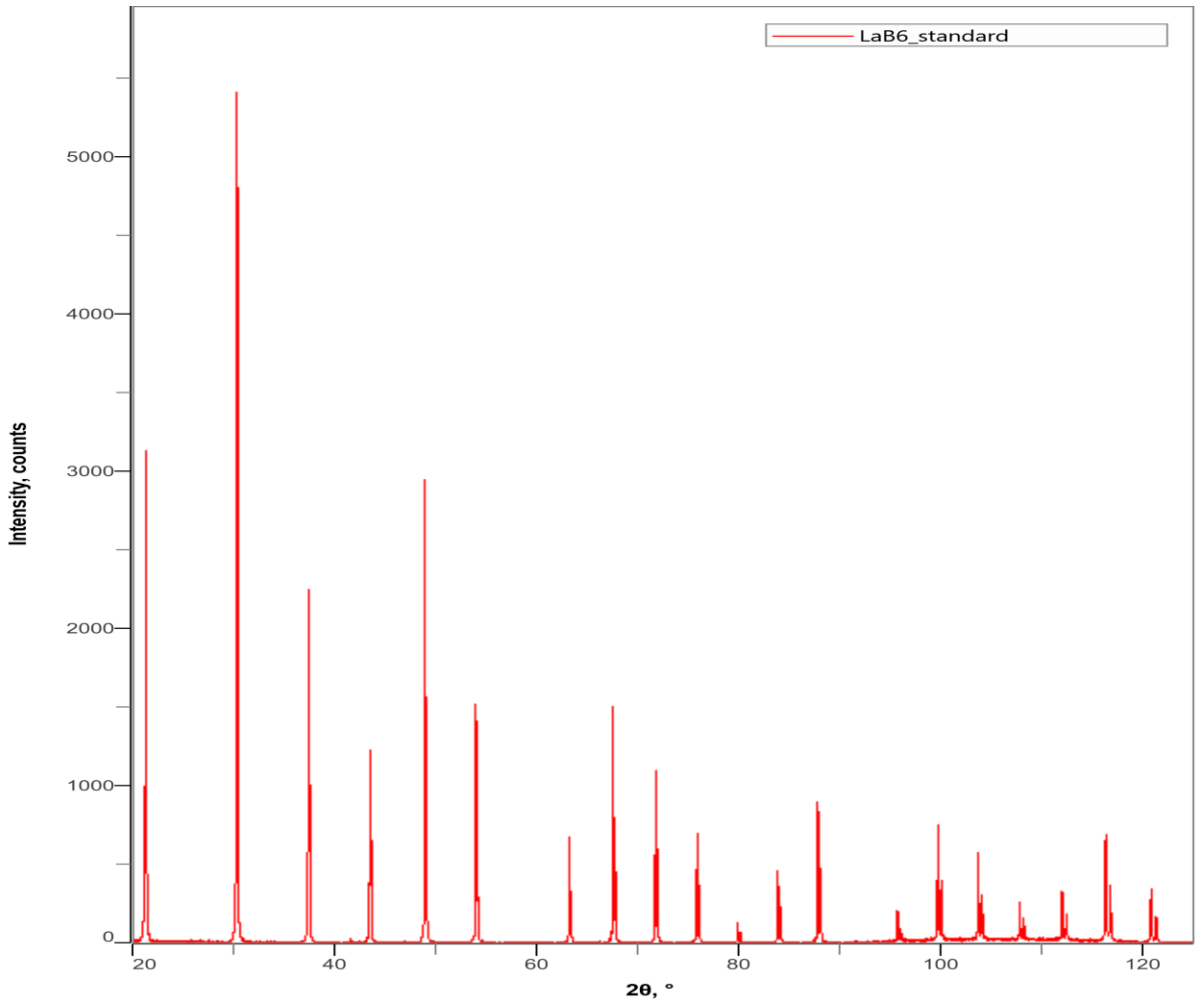
General information

Analysis date	2026-02-22 13:24:16	Measurement start time	2010-04-28 07:31:00
Analyst	Administrator	Operator	
Sample name	LaB6-660a	Comment	Crystal Size (Ext)
Measured data name	C:\Dr. Butt\DemoData\Manuals\PowderXRD\Basic\LaB6_standard.rasx	Memo	LaB6-660a

Measurement Conditions

X-Ray generator	45 kV, 40 mA	Scan mode	0D(step)
Incident primary	None	Scan speed/Duration time	0.50 s
Goniometer	Ultima IV (Protectus)	Step width	0.01 °
Attachment	None	Scan axis	θ/2θ
Filter	10 mm	Scan range	20 ~ 125 °
Selection slit	None	Incident slit box	1deg.
Diffracted beam mono	Fixed Monochromator(U4)	Length-limiting slit	None
Detector	Scintillation counter	Receiving slit box #1	1deg.
Optics attribute	None	Receiving slit box #2	0.15 mm

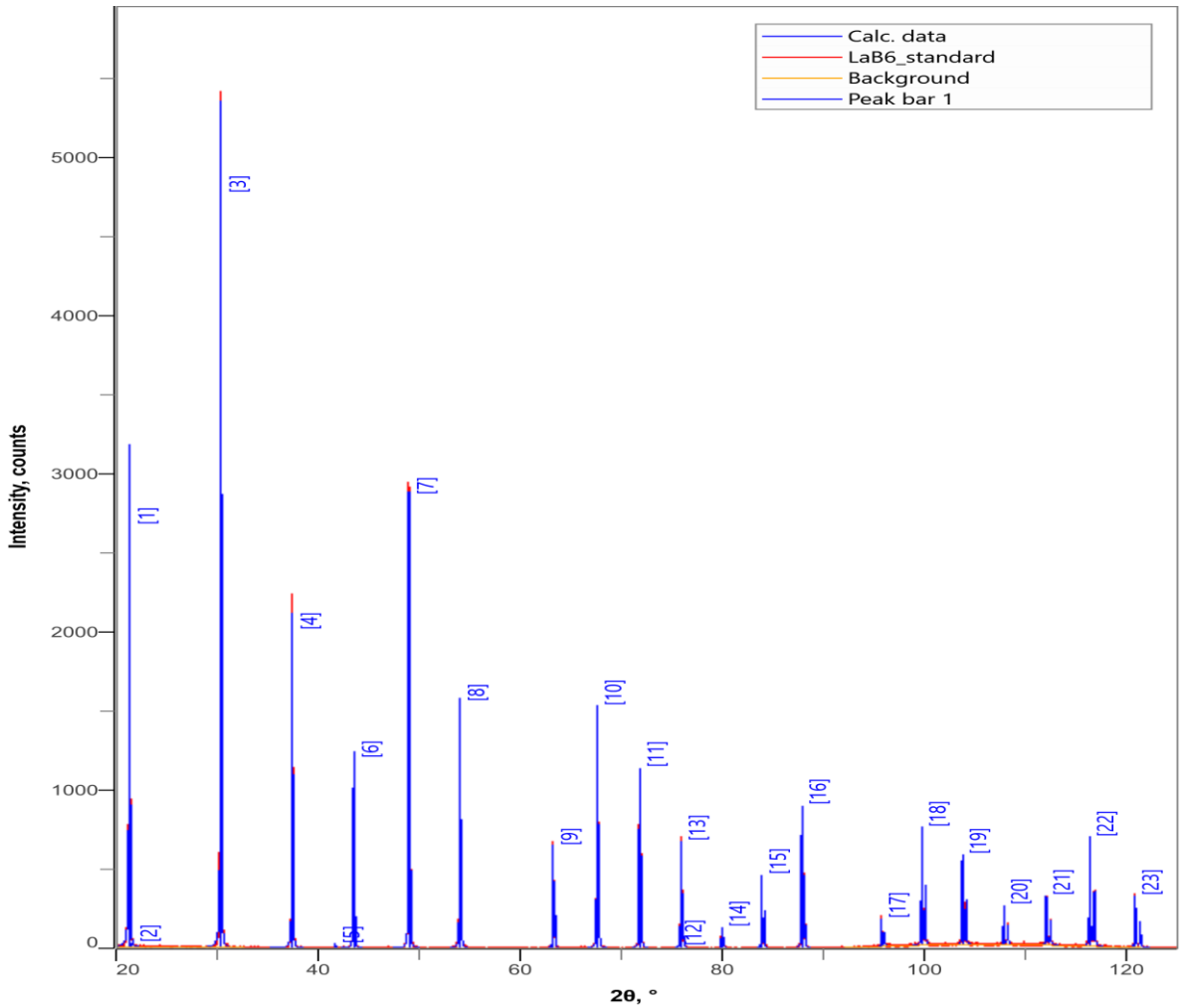
Measured profile view



Peak evaluation conditions

Peak search method	Second derivative method	σ cut	3.00		
Profile fitting	Run completed	Peak shape	Split pseudo-Voigt	Fitting condition	Auto(Refine background)

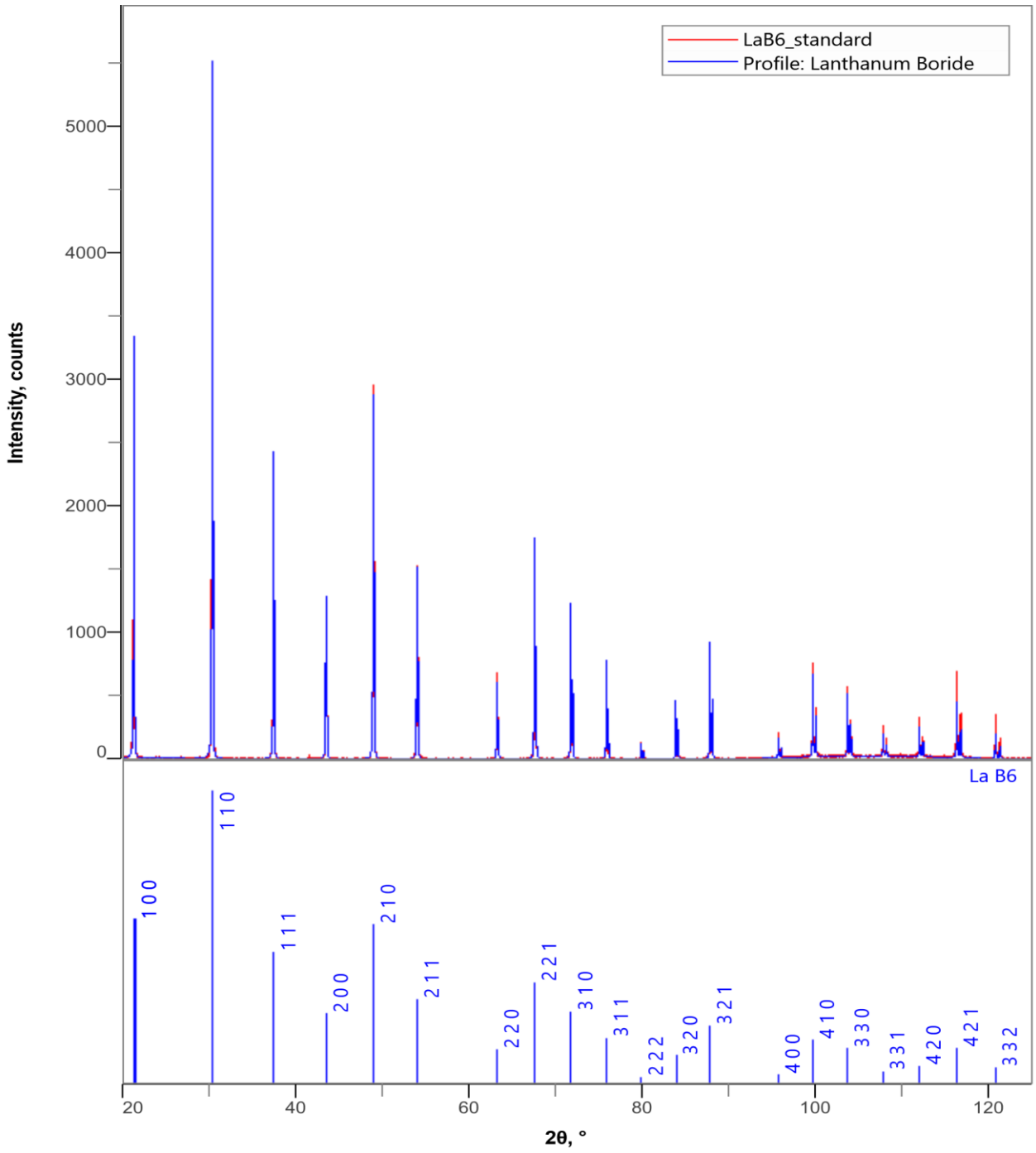
Peak Profile View



Qualitative Analysis Results

Phase name	Chemical formula	FOM	Phase reg. detail	Space Group	DB Card Number
Lanthanum Boride	La B6	0.204	S/M:PDF-2 2026	221 : Pm-3m	00-059-0332

Phase Data View



Peak list

No.	2θ, °	d, Å	FWHM, °	Size, Å	Phase Name	Chemical Formula	Card No	Strain, %
1	21.3260(11)	4.1629(2)	0.0706(18)	1196(31)	Lanthanum Boride: 1 0 0	La B6	00-059-0332	-
2	21.57(2)	4.117(4)	0.13(5)	647(261)	Unknown			-
3	30.3613(19)	2.94153(18)	0.080(2)	1070(27)	Lanthanum Boride: 1 1 0	La B6	00-059-0332	-
4	37.4255(18)	2.40094(11)	0.0762(16)	1150(24)	Lanthanum Boride: 1 1 1	La B6	00-059-0332	-
5	41.620(4)	2.16817(18)	0.050(13)	1772(451)	Unknown			-
6	43.4914(14)	2.07910(6)	0.0708(12)	1261(21)	Lanthanum Boride: 2 0 0	La B6	00-059-0332	-
7	48.9451(12)	1.85942(4)	0.0706(10)	1292(18)	Lanthanum Boride: 2 1 0	La B6	00-059-0332	-
8	53.9777(15)	1.69734(4)	0.0705(14)	1320(26)	Lanthanum Boride: 2 1 1	La B6	00-059-0332	-
9	63.2091(18)	1.46985(4)	0.0716(17)	1361(32)	Lanthanum Boride: 2 2 0	La B6	00-059-0332	-
10	67.5373(13)	1.38579(2)	0.0724(12)	1379(23)	Lanthanum Boride: 2 2 1	La B6	00-059-0332	-
11	71.7344(14)	1.31468(2)	0.0728(13)	1407(25)	Lanthanum Boride: 3 1 0	La B6	00-059-0332	-
12	75.463(7)	1.25870(10)	0.051(17)	2072(684)	Unknown			-
13	75.8365(19)	1.25343(3)	0.0773(17)	1360(30)	Lanthanum Boride: 3 1 1	La B6	00-059-0332	-
14	79.859(4)	1.20010(5)	0.076(4)	1422(69)	Lanthanum Boride: 2 2 2	La B6	00-059-0332	-
15	83.835(2)	1.15301(3)	0.077(2)	1448(39)	Lanthanum Boride: 3 2 0	La B6	00-059-0332	-

16	87.7865(17)	1.111007(17)	0.0804(15)	1431(27)	Lanthanum Boride: 3 2 1	La B6	00-059-0332	-
17	95.664(4)	1.03926(3)	0.078(4)	1585(80)	Lanthanum Boride: 4 0 0	La B6	00-059-0332	-
18	99.6407(19)	1.008186(14)	0.0885(17)	1452(28)	Lanthanum Boride: 4 1 0	La B6	00-059-0332	-
19	103.657(3)	0.979797(17)	0.089(2)	1516(41)	Lanthanum Boride: 3 3 0	La B6	00-059-0332	-
20	107.752(4)	0.95362(2)	0.089(4)	1577(74)	Lanthanum Boride: 3 3 1	La B6	00-059-0332	-
21	111.933(3)	0.929493(18)	0.100(3)	1477(46)	Lanthanum Boride: 4 2 0	La B6	00-059-0332	-
22	116.247(2)	0.907076(11)	0.100(2)	1568(34)	Lanthanum Boride: 4 2 1	La B6	00-059-0332	-
23	120.731(3)	0.886199(14)	0.110(3)	1524(43)	Lanthanum Boride: 3 3 2	La B6	00-059-0332	-

Lattice parameters

Phase name	a, Å	b, Å	c, Å	α, °	β, °	γ, °
Lanthanum Boride	4.15592	4.15592	4.15592	90.000	90.000	90.000

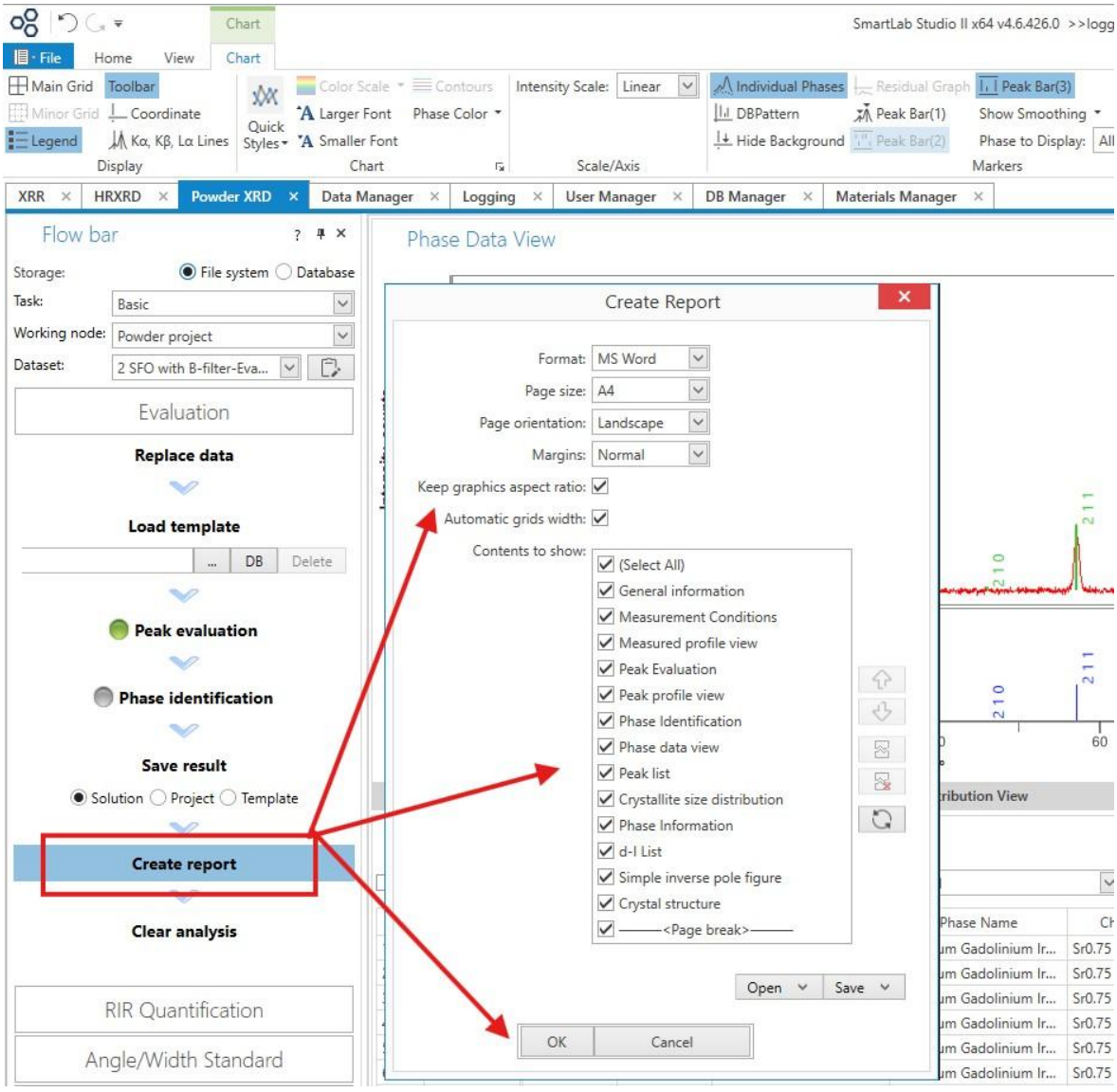
d-I List

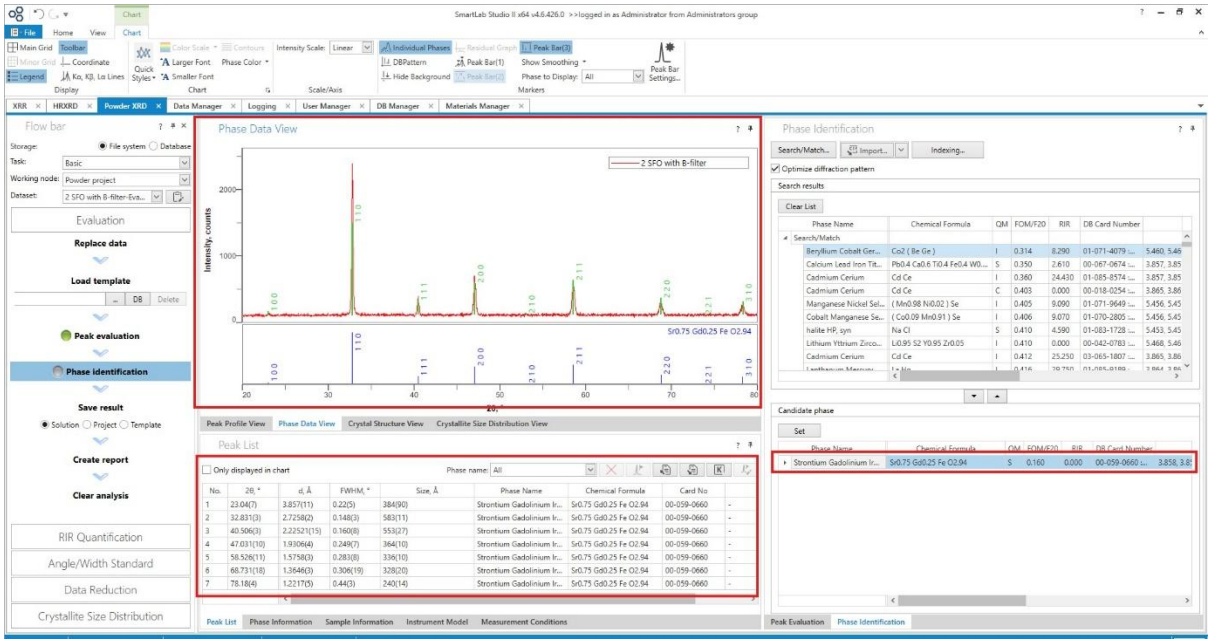
Lanthanum Boride

No.	2θ, °	d, Å	h k l	Norm. I.
1	21.36250	4.15592	1 0 0	55.80
2	30.39148	2.93868	1 1 0	100.00
3	37.45009	2.39942	1 1 1	45.00
4	43.51636	2.07796	2 0 0	24.10
5	48.96863	1.85859	2 1 0	54.40
6	54.00132	1.69665	2 1 1	29.00
7	63.23351	1.46934	2 2 0	11.90
8	67.56408	1.38531	3 0 0	0.00
9	67.56408	1.38531	2 2 1	34.80
10	71.76324	1.31422	3 1 0	24.80
11	75.86315	1.25306	3 1 1	15.90

12	79.89031	1.19971	2 2 2	2.60
13	83.86752	1.15265	3 2 0	9.70
14	87.81524	1.11072	3 2 1	20.00
15	95.69823	1.03898	4 0 0	3.40
16	99.67124	1.00796	4 1 0	15.20
17	99.67124	1.00796	3 2 2	0.00
18	103.69186	0.97956	4 1 1	0.00
19	103.69186	0.97956	3 3 0	12.20
20	107.78258	0.95343	3 3 1	4.60
21	111.96940	0.92929	4 2 0	6.40
22	116.28375	0.90690	4 2 1	12.50
23	120.76529	0.88605	3 3 2	5.80

Report of the sample SFO





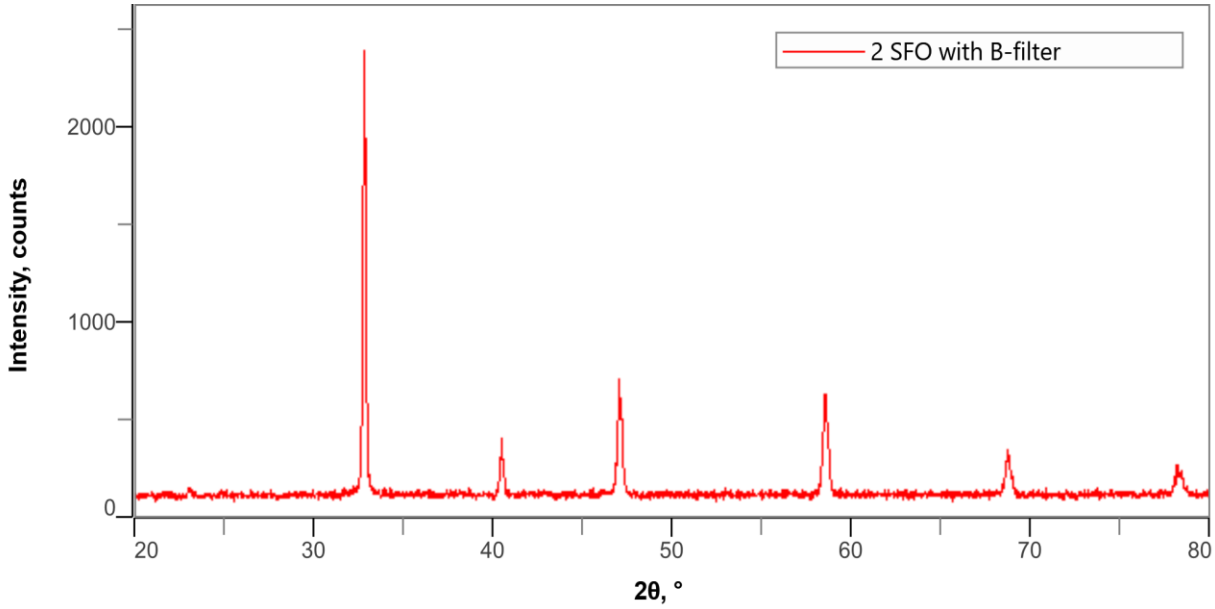
General information

Analysis date	2026-01-29 17:23:08	Measurement start time	2025-12-16 09:51:29
Analyst	Administrator	Operator	Administrator
Sample name		Comment	
Measured data name	C:\Dr. Butt\2 SFO with B-filter.rasx	Memo	

Measurement Conditions

X-Ray generator	40 kV, 45 mA	Scan mode	1D(scan)
Incident primary	Standard	Scan speed/Duration time	4.00 °/min
Goniometer	Standard Goniometer	Step width	0.02 °
Attachment	Standard attachment head	Scan axis	θ/2θ
Filter	Kβ filter 1D for Cu	Scan range	20 ~ 80 °
Selection slit	BB	Incident slit box	1deg
Diffracted beam mono	None	Length-limiting slit	10 mm
Detector	D/teX Ultra 250	Receiving slit box #1	1.000mm
Optics attribute	BB	Receiving slit box #2	1.125mm

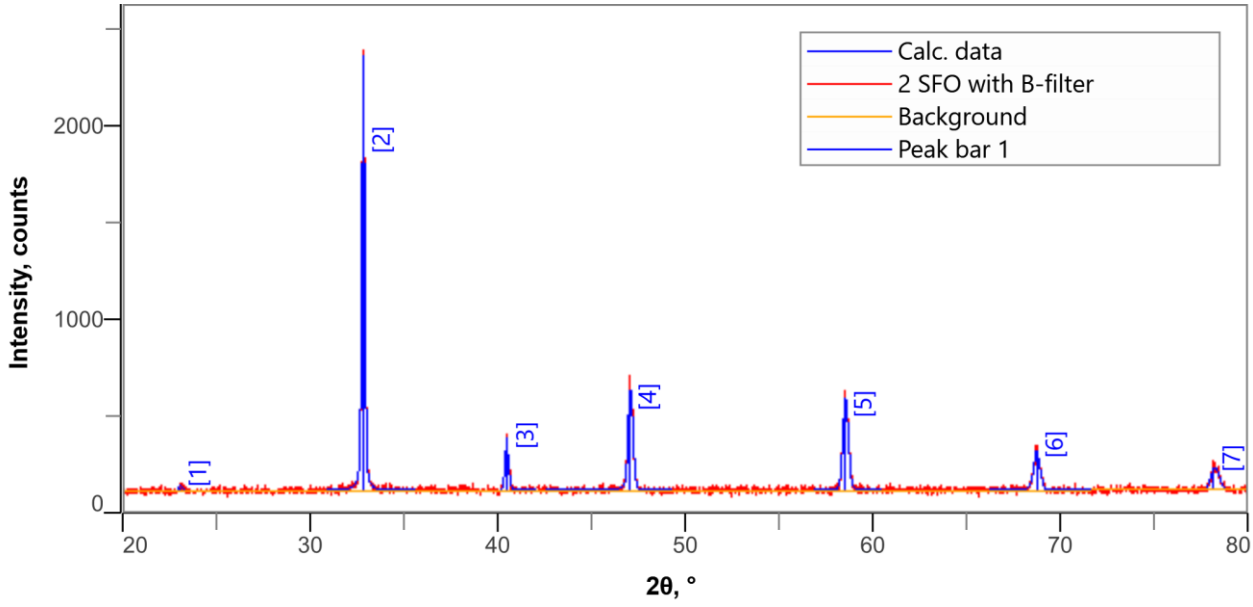
Measured profile view



Peak evaluation conditions

Peak search method	Second derivative method	σ cut	3.00		
Profile fitting	Run completed	Peak shape	Split pseudo-Voigt	Fitting condition	Auto(Refine background)

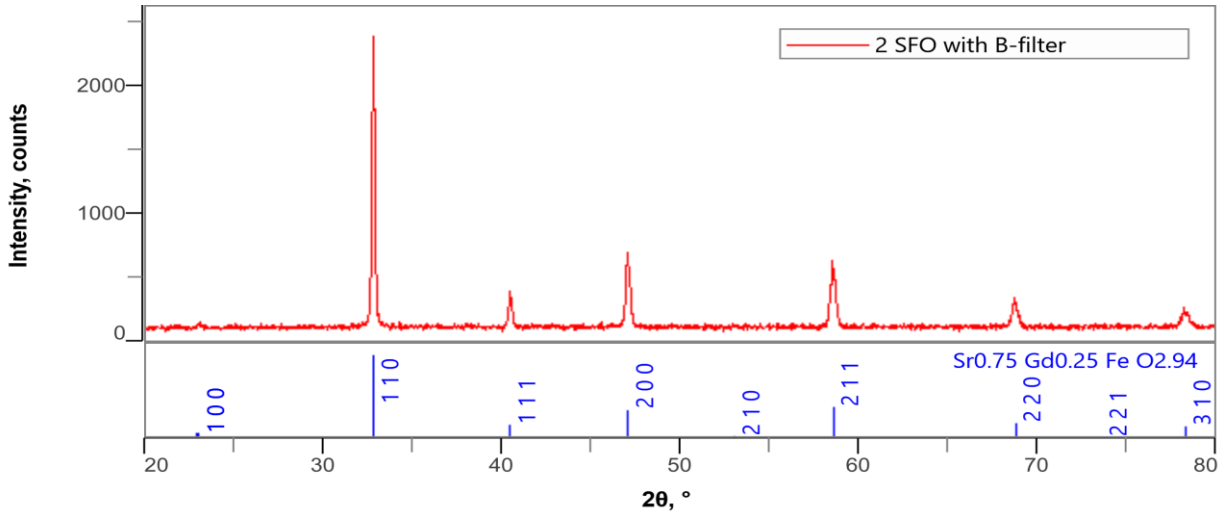
Peak Profile View



Qualitative Analysis Results

Phase name	Chemical formula	FOM	Phase reg. detail	Space Group	DB Card Number
Strontium Gadolinium Iron Oxide	Sr0.75 Gd0.25 Fe O2.94	0.160	S/M:PDF-2 2026	221 : Pm-3m	00-059-0660

Phase Data View



Peak list

No.	2θ, °	d, Å	FWHM, °	Size, Å	Phase Name	Chemical Formula	Card No
1	23.04(7)	3.857(11)	0.22(5)	384(90)	Strontium Gadolinium Iron Oxide: 1 0 0	Sr0.75 Gd0.25 Fe O2.94	00-059-0660
2	32.831(3)	2.7258(2)	0.148(3)	583(11)	Strontium Gadolinium Iron Oxide: 1 1 0	Sr0.75 Gd0.25 Fe O2.94	00-059-0660
3	40.506(3)	2.22521(15)	0.160(8)	553(27)	Strontium Gadolinium Iron Oxide: 1 1 1	Sr0.75 Gd0.25 Fe O2.94	00-059-0660
4	47.031(10)	1.9306(4)	0.249(7)	364(10)	Strontium Gadolinium Iron Oxide: 2 0 0	Sr0.75 Gd0.25 Fe O2.94	00-059-0660
5	58.526(11)	1.5758(3)	0.283(8)	336(10)	Strontium Gadolinium Iron Oxide: 2 1 1	Sr0.75 Gd0.25 Fe O2.94	00-059-0660
6	68.731(18)	1.3646(3)	0.306(19)	328(20)	Strontium Gadolinium Iron Oxide: 2 2 0	Sr0.75 Gd0.25 Fe O2.94	00-059-0660
7	78.18(4)	1.2217(5)	0.44(3)	240(14)	Strontium Gadolinium Iron Oxide: 3 1 0	Sr0.75 Gd0.25 Fe O2.94	00-059-0660

Lattice parameters

Phase name	a, Å	b, Å	c, Å	α, °	β, °	γ, °
Strontium Gadolinium Iron Oxide	3.85758	3.85758	3.85758	90.000	90.000	90.000

d-I List

Strontium Gadolinium Iron Oxide

No.	2θ, °	d, Å	h k l	Norm. I.
1	23.03697	3.85758	1 0 0	4.50
2	32.80651	2.72772	1 1 0	100.00
3	40.46897	2.22717	1 1 1	16.20
4	47.07738	1.92879	2 0 0	36.90
5	53.03962	1.72516	2 1 0	2.10
6	58.56606	1.57485	2 1 1	41.90
7	68.77569	1.36386	2 2 0	21.60
8	73.60411	1.28586	3 0 0	0.00
9	73.60411	1.28586	2 2 1	1.10
10	78.31534	1.21987	3 1 0	17.80

Candidate selection rules of thumb

1. **Start with the phase that explains the strongest peaks**

   The first candidate should account for the highest-intensity measured peaks (not just many weak ones).

2. **Require "multi-peak proof"**

   A valid candidate should match several reflections across the scan range, not 1–2 coincidences.

3. **Reject phases that predict "missing strong peaks"**

   If the reference pattern has strong lines that are clearly absent in the measured pattern (and not masked), do not select it.

4. **Use peak positions as the primary filter**

   For qualitative ID, 2θ/d agreement matters more than intensity. Intensity can change due to texture, absorption, and microstructure.

5. **Check for systematic 2θ shift vs random mismatch**

   If most peaks match but are shifted together, that may indicate zero shift / **displacement** or **lattice parameter difference** (solid solution).

   If mismatches are random, it's likely the wrong phase.

6. **Prefer candidates that reduce the "unassigned peaks"**

Add a candidate only if it explains peaks that remain unexplained after previous candidates.

7. **Avoid overfitting weak/noisy features**

   Don't add a new candidate just to explain one tiny peak near the noise floor unless it is chemically expected and repeatable.

8. **Give priority to chemically/plausibly reachable phases**

   Prefer phases consistent with sample chemistry, synthesis route, processing temperature, atmosphere, and known impurities.

9. **Be careful if the background is high or noisy**

   A high background (often from fluorescence, poor counting, or sample issues) can hide real peaks and create false peak picks. In such cases, rely more on clear peak positions and re-check with better preprocessing or a different source/filter if needed.

10. **Use "phase family" logic**

    When multiple results are closely related (polymorphs/solid solutions), pick the one that best matches peak positions and eliminates conflicts, then treat others as alternates.

11. **Check low-angle region and high-angle region**

    A good candidate typically matches at both low and high 2θ; matching only one region is a warning sign.

12. **Don't reject a phase only because intensities look different**

    If peak *positions* match well but the *relative intensities* don't, the phase may still be correct because preferred orientation (texture), absorption, or microstructure can change intensities. Keep it as a candidate and note texture as a likely reason.

13. **Avoid selecting two candidates that represent the same phase**

    Many database hits can be very similar (same phase with different cards or closely related variants) and will explain the same peaks. Choose the one that fits best and only keep multiple similar candidates if there is clear evidence that two nearly identical phases are truly present.

14. **Stop adding candidates when conflicts increase**

    Candidate building should reduce residual unexplained peaks without creating new missing-peak conflicts. If adding a phase increases contradictions, remove it.

15. **Final sanity check**

    After candidate selection, confirm:

    - No major measured peaks are left unexplained
    - No candidate has strong predicted peaks missing
    - The set is chemically reasonable and minimal (as few phases as needed)