



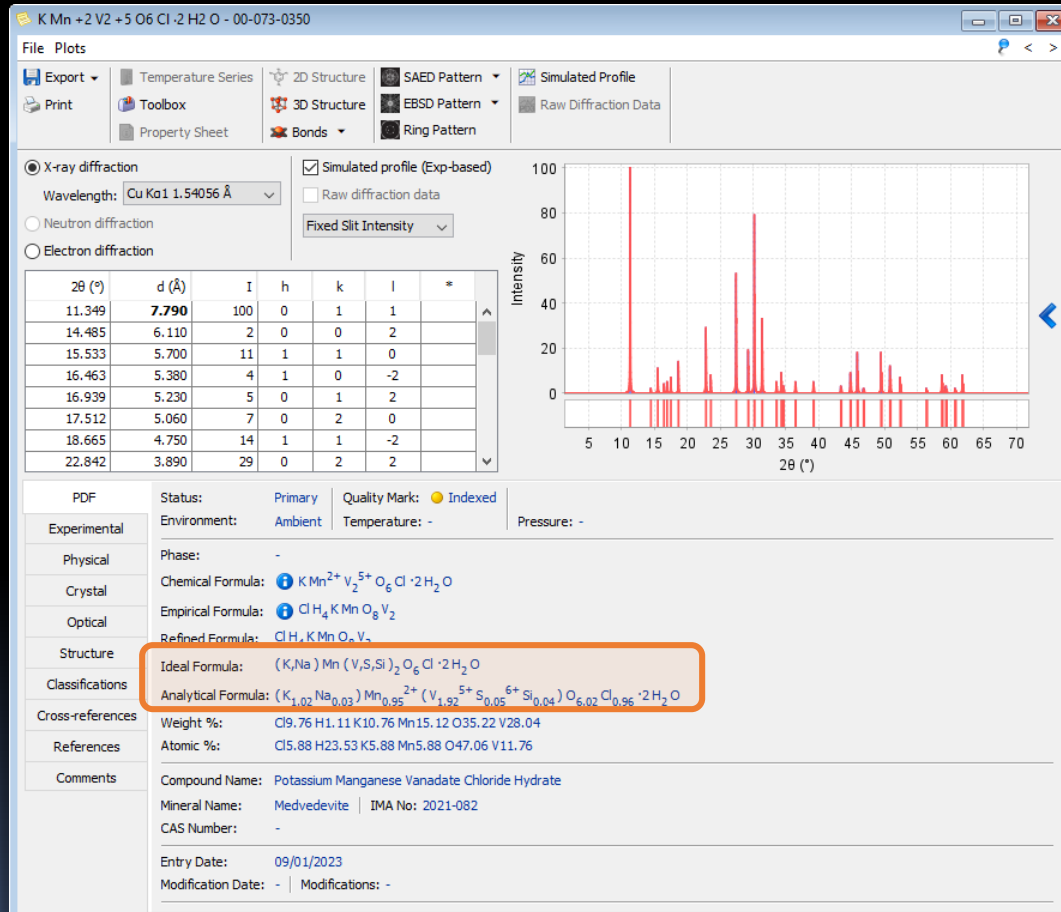
New Features for Release 2024

PDF-5+ 2024 Database



- PDF-4+ and PDF-4/Organics have been combined into a single database
- Contains 1,061,898 entries
- Use both sets of data simultaneously or individually

New Formula Fields



Ideal Formula

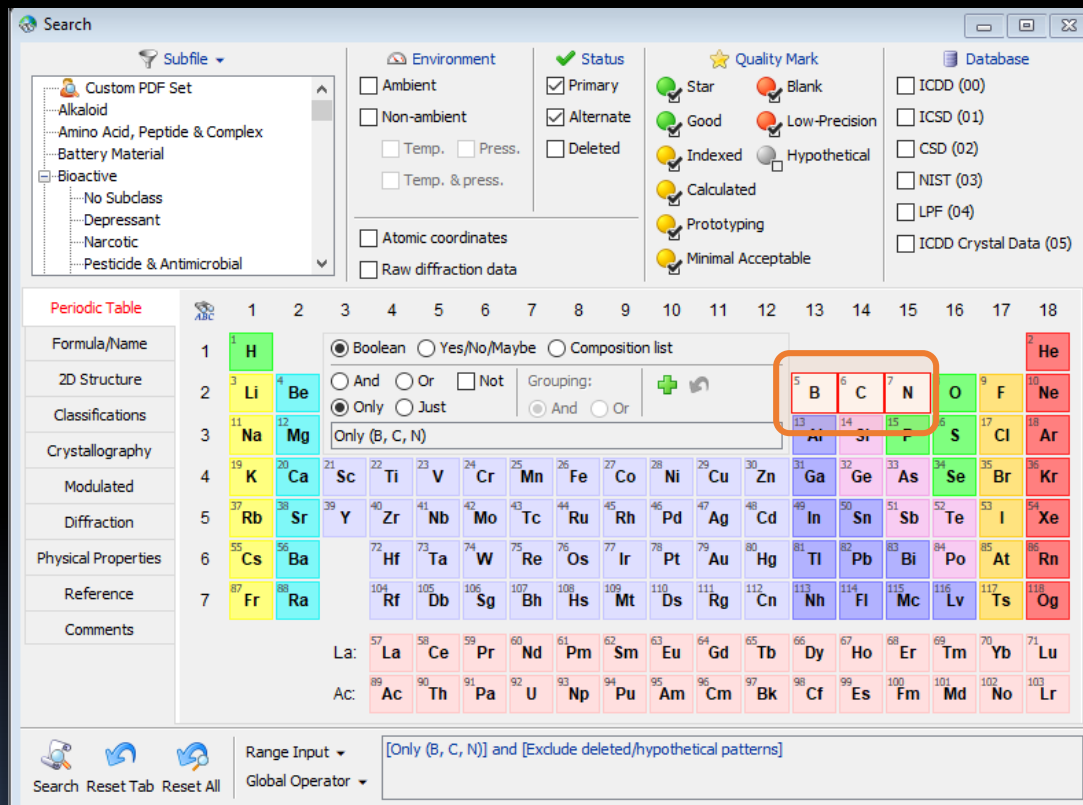
- Describes the general chemistry of the compound, especially in cases of minerals and solid solutions. Minor substituents or variations may be ignored in this representation.

Analytical Formula

- Based on experimental elemental analysis, such as XRF and microprobe analysis. This formula is descriptive and represents a composition derived based on experimental measurements.

PDF card with the new Ideal Formula and Analytical Formula fields

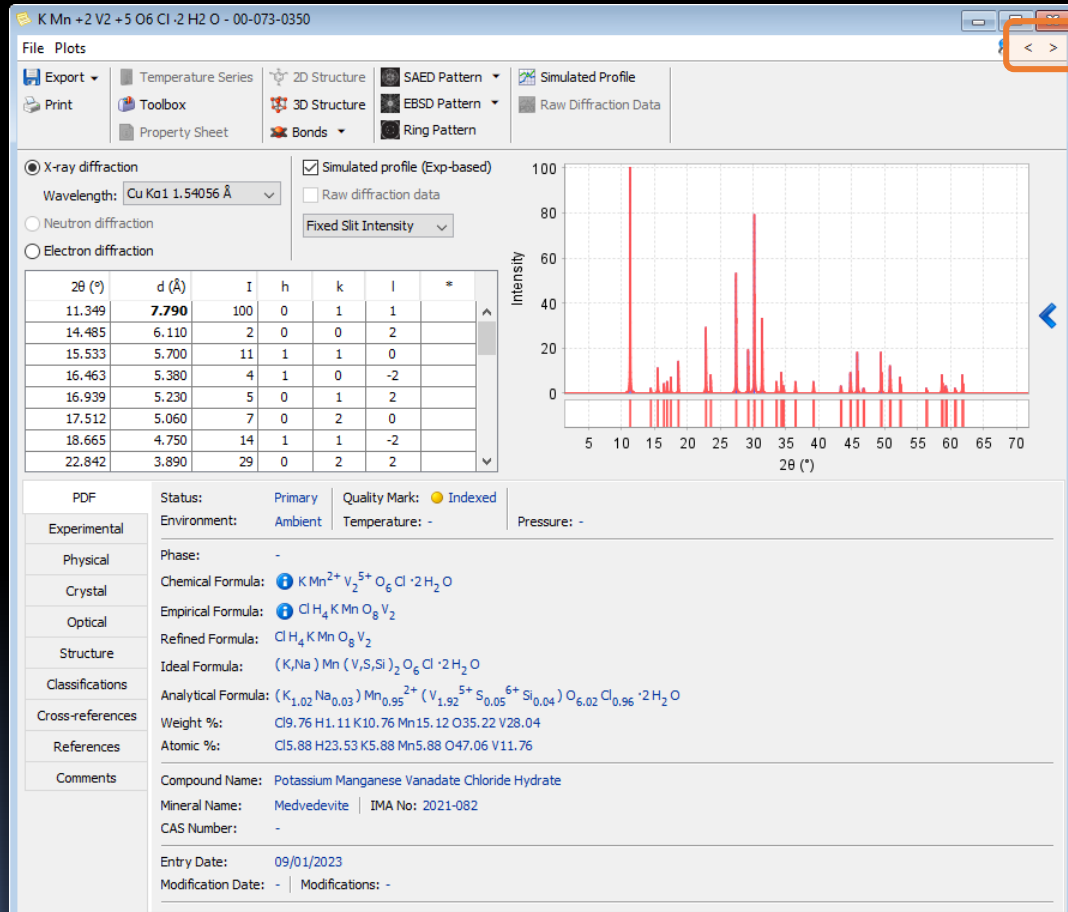
Optimized Element Searches



The “Only” and “Just” operators for the periodic table search have been optimized for faster results

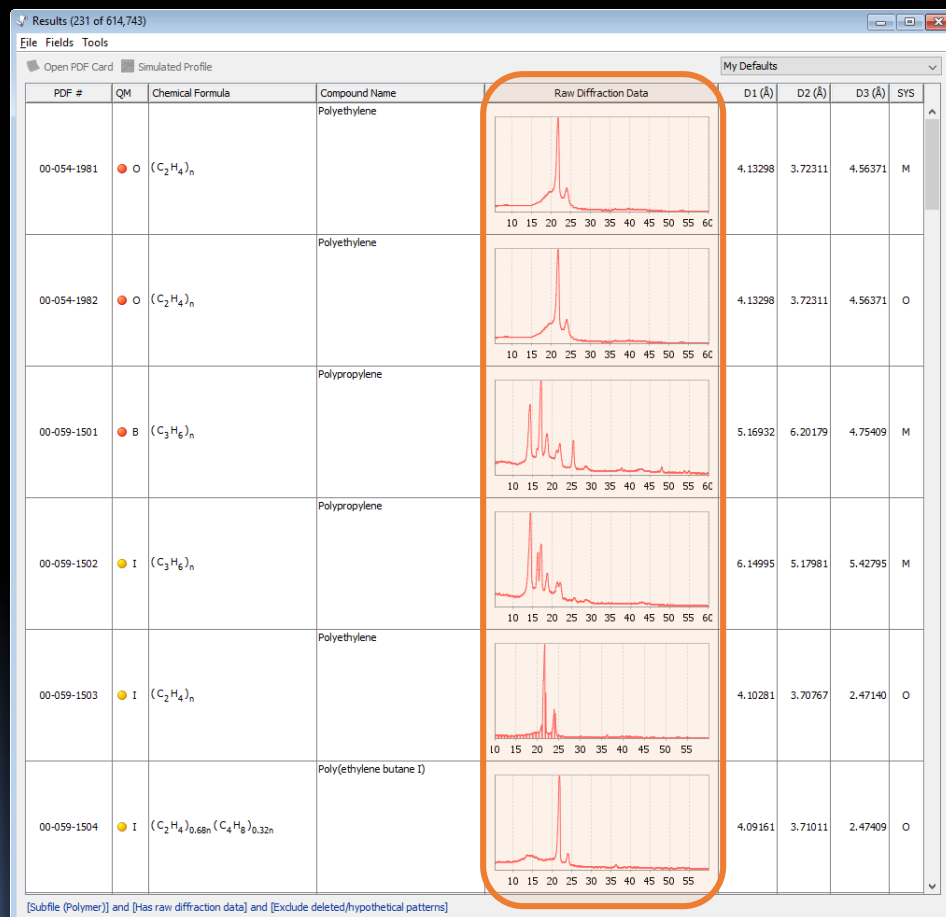
	2023	2024
Only (B, C, N)	2.6s	0.5s
Just (H, C, N, P, O)	45.5s	7.3s
Just (Mg, B, Al, C, Si, N, O, F)	2m 38s	1s

PDF Card Features



- New arrow buttons allow the user to quickly traverse through the search results table
 - Mouse wheel option

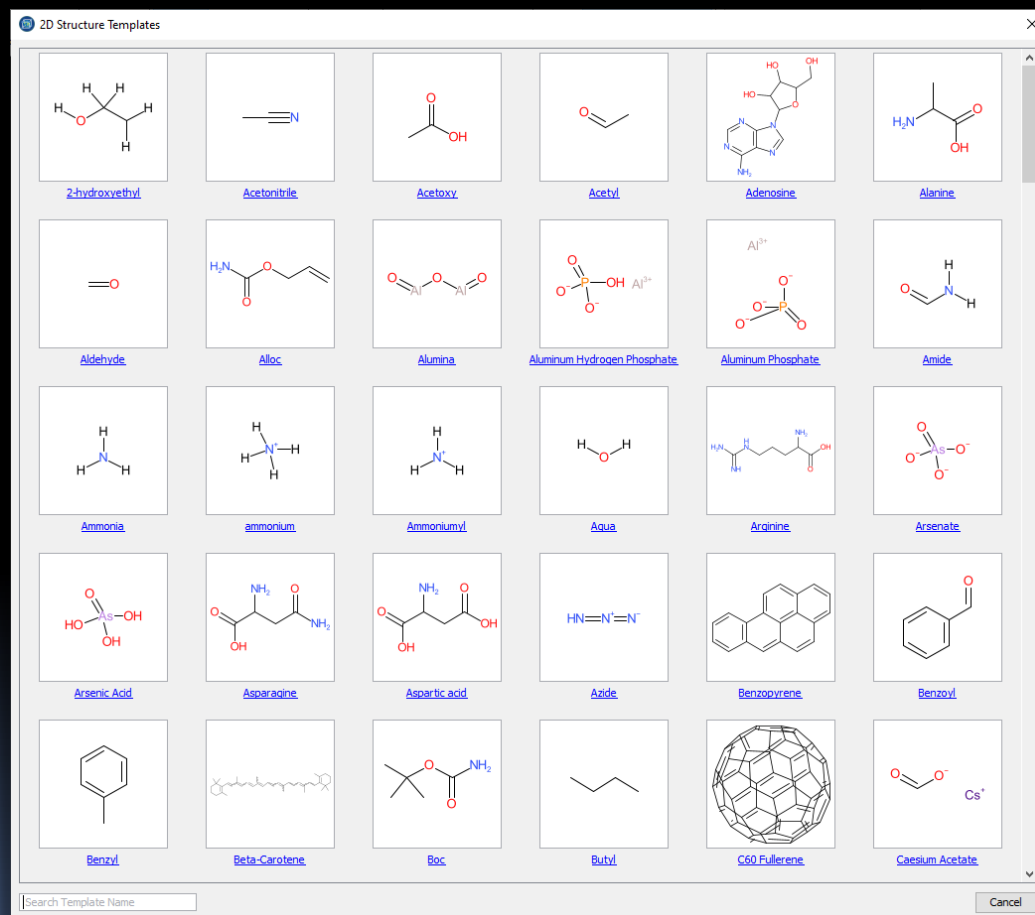
Graphing Features



- Automatic vertical zooming
- Gradient color fill option
- Raw data (PD3 patterns) in search results*
- Diffraction pattern preview when dragging and dropping*

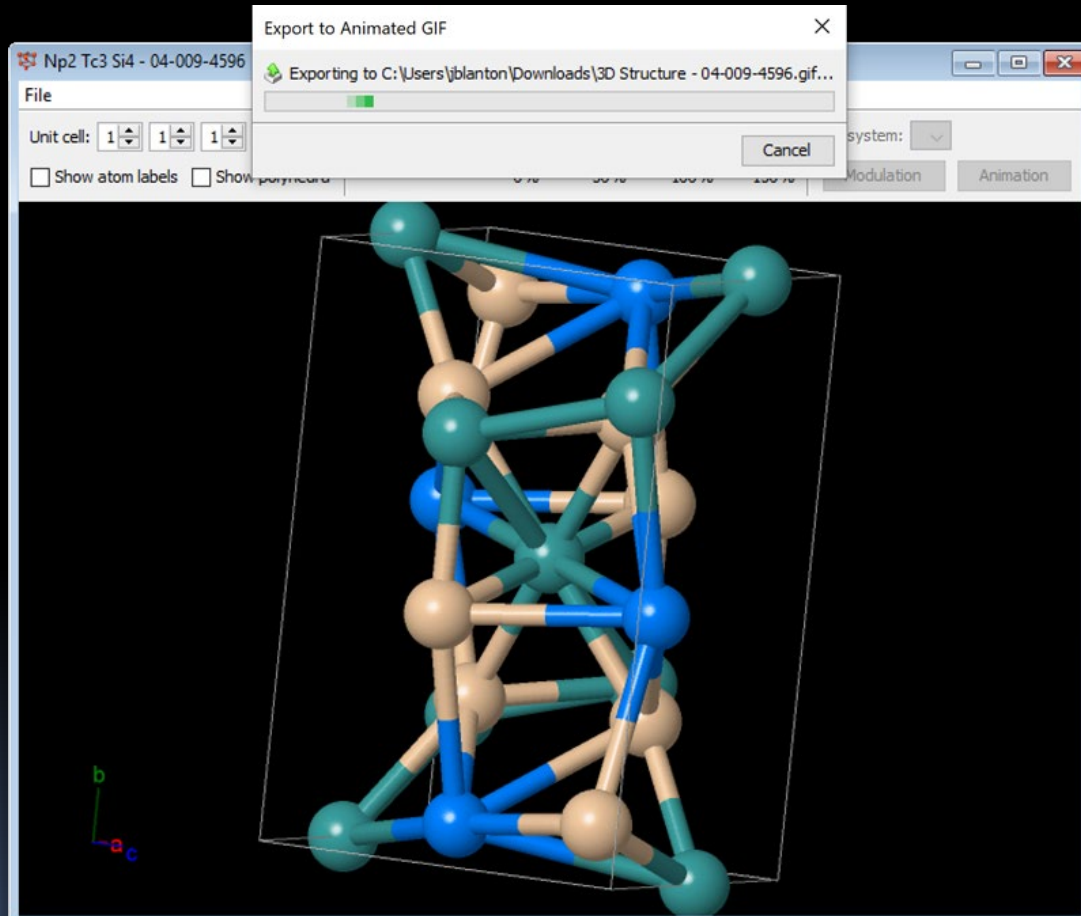
Search results with raw data (PD3 patterns)

2D Structure Templates*



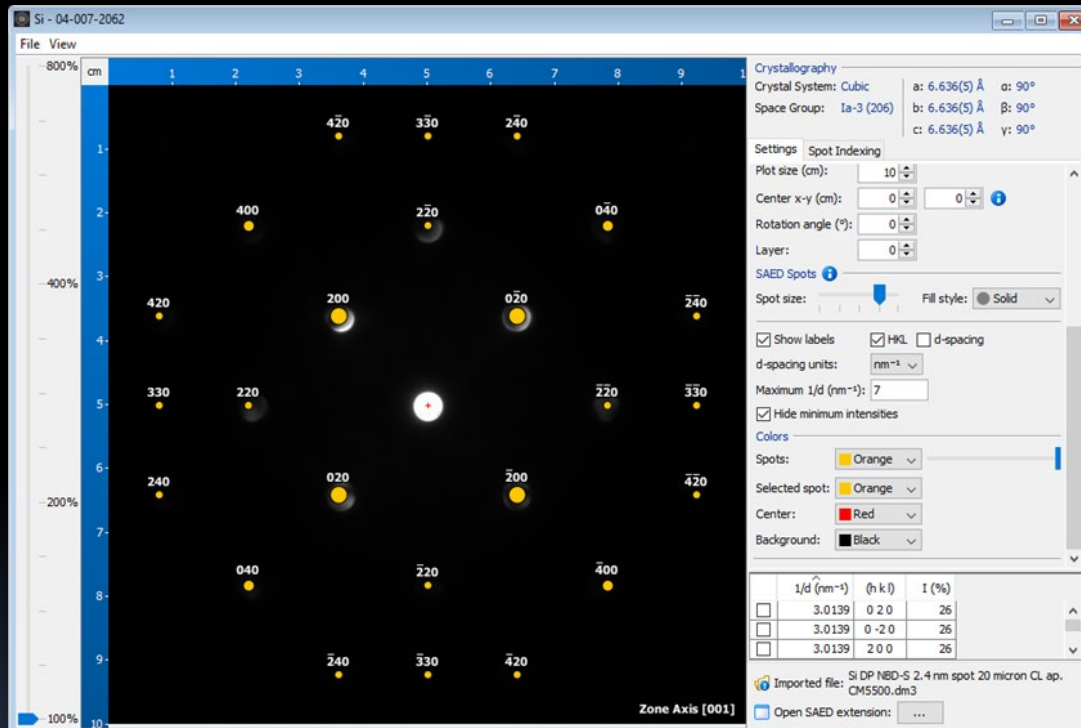
- Used for 2D structure and substructure searches
- 200 templates available
- Use as starting structure or complete structure
- Search by template name

3D Structure Features*



- Export 3D structure animation to a GIF file

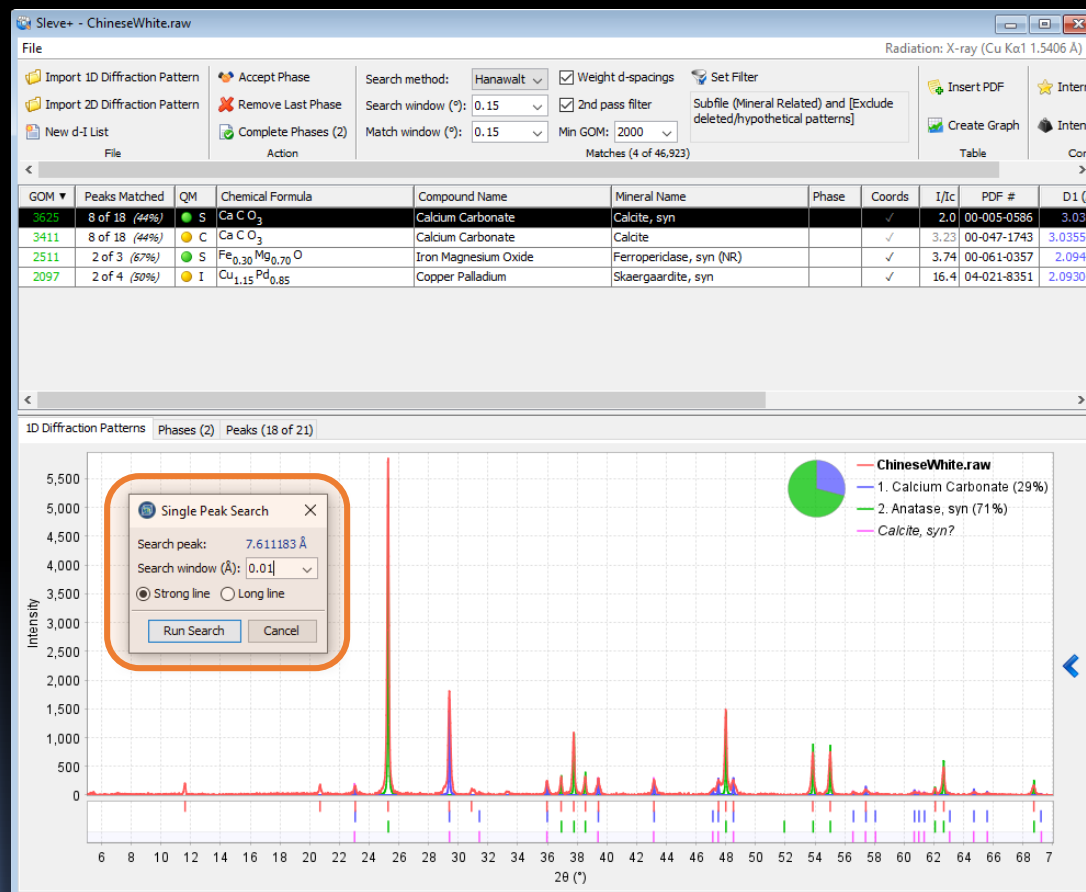
SAED Simulation Features*



Imported Gatan *.dm3 image overlay on SAED simulation of silicon

- Added support for importing Gatan *.dm3 files
- Fill style for spots
 - Gradient
 - Solid

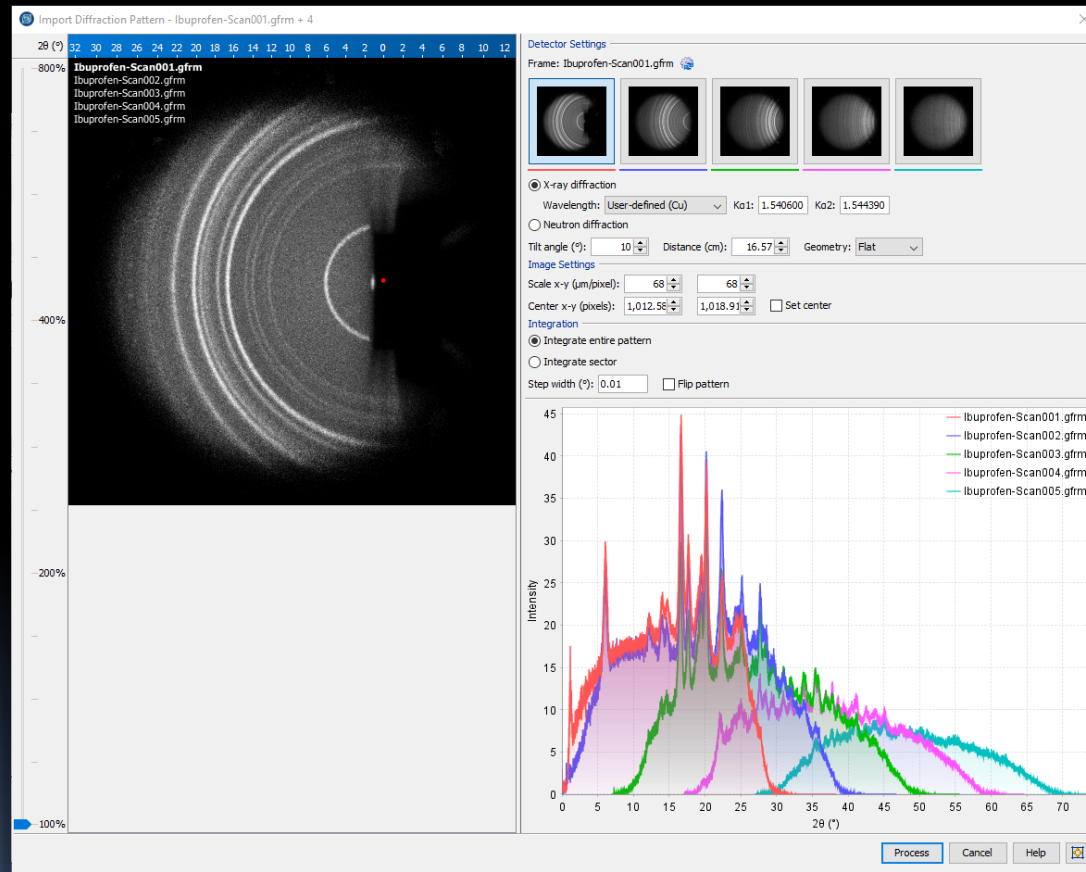
Sieve/Sieve+ Features



- Support for new file formats
 - Rigkau *.asc
 - Rigkau *.rasx
- Hide irrelevant matches
- Supports NIST SRM 660c as an internal standard
- Single peak search
 - Select peak using the mouse
 - Search strong or long lines
 - User-defined error window
 - Useful for trace phase analysis

Sieve+ with new single peak search feature (for trace phase analysis)

2D Diffraction Features*



- 2D images are dynamically displayed when importing multiple files
- Red vertical line indicates progress of pattern integration
- Thumbnail preview images

Importing five 2D diffraction pattern “frames” into Sleve+ for phase ID