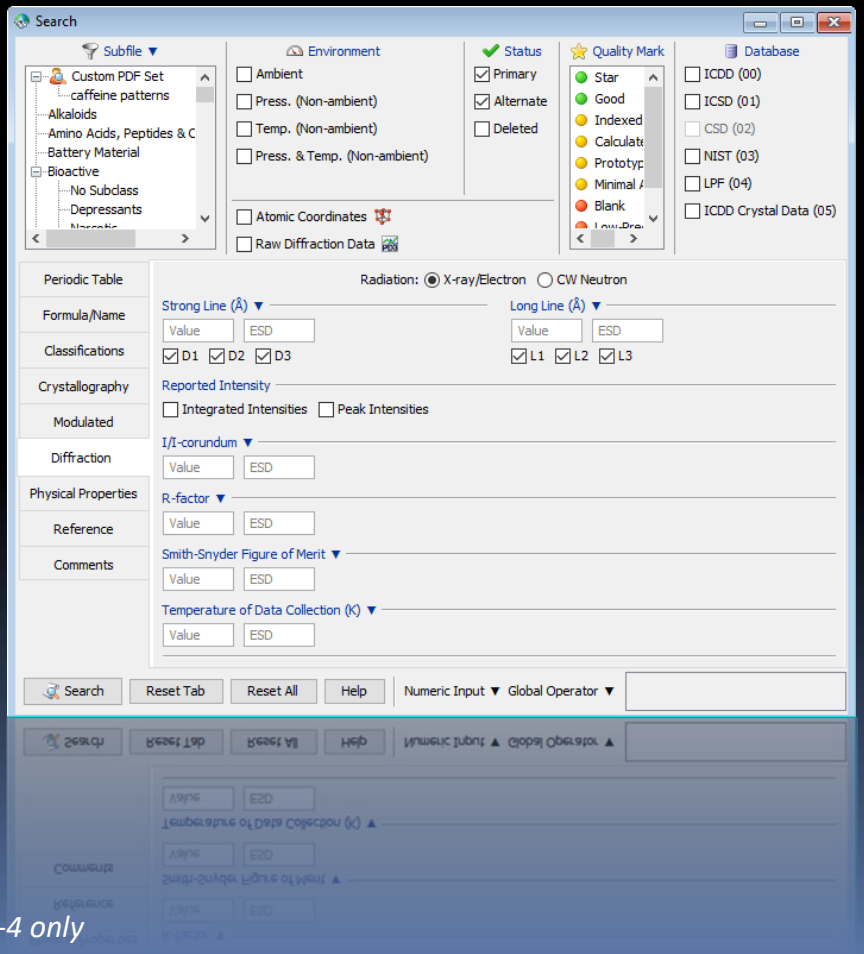
NEW FEATURES FOR RELEASE 2018

New Features for Release 2018

The 2018 release of ICDD databases boasts an impressive array of new features. This tutorial will show these new features using ICDD's own data mining software, which is bundled free with the database. These features include:

- Data Mining Enhancements
- PDF Card Enhancements
- Graphing Enhancements
- New Pattern Simulation Features
- Sleve+ Improvements
- Neutron Diffraction Enhancements

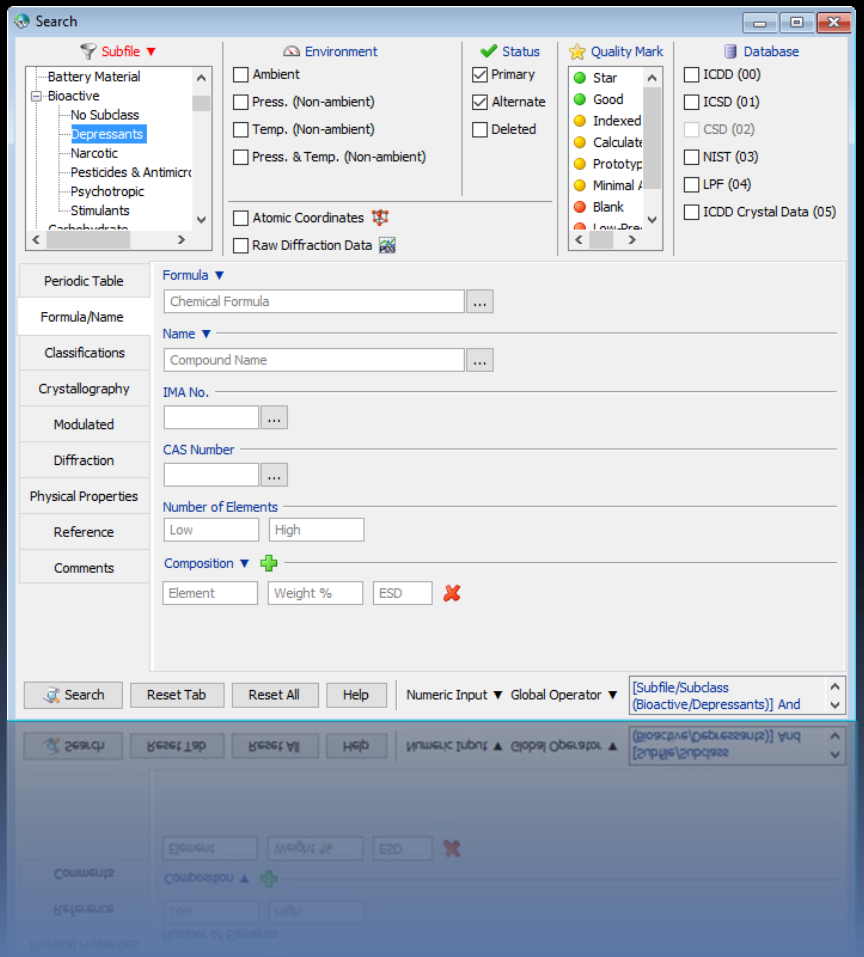
Data Mining



- Reported Intensity search
  - Peak Intensities
  - Integrated Intensities
- Subfiles display field*
- Metals & Alloys – Standard Index*
  - Based on the accepted Linus Pauling File (LPF) prototype structure for each material
  - Empirical Formula [Std.]
  - Space Group
  - Z [Std.]
  - Wyckoff Seq. [Std.]

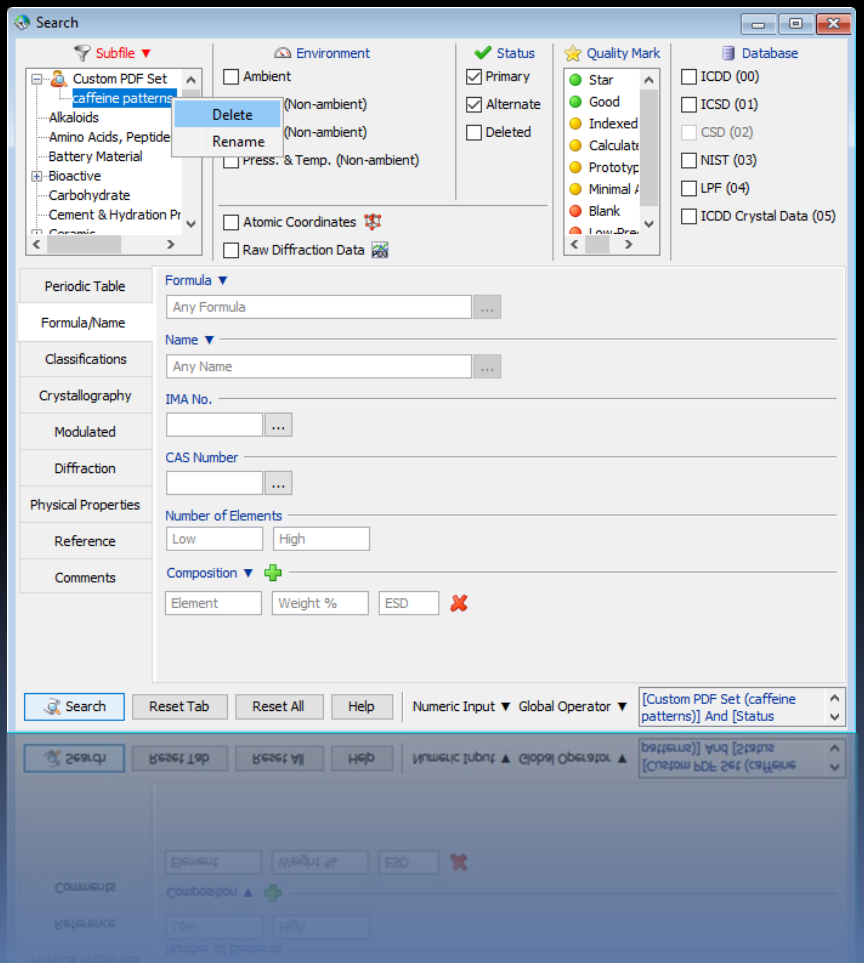
*PDF-4 only

Data Mining



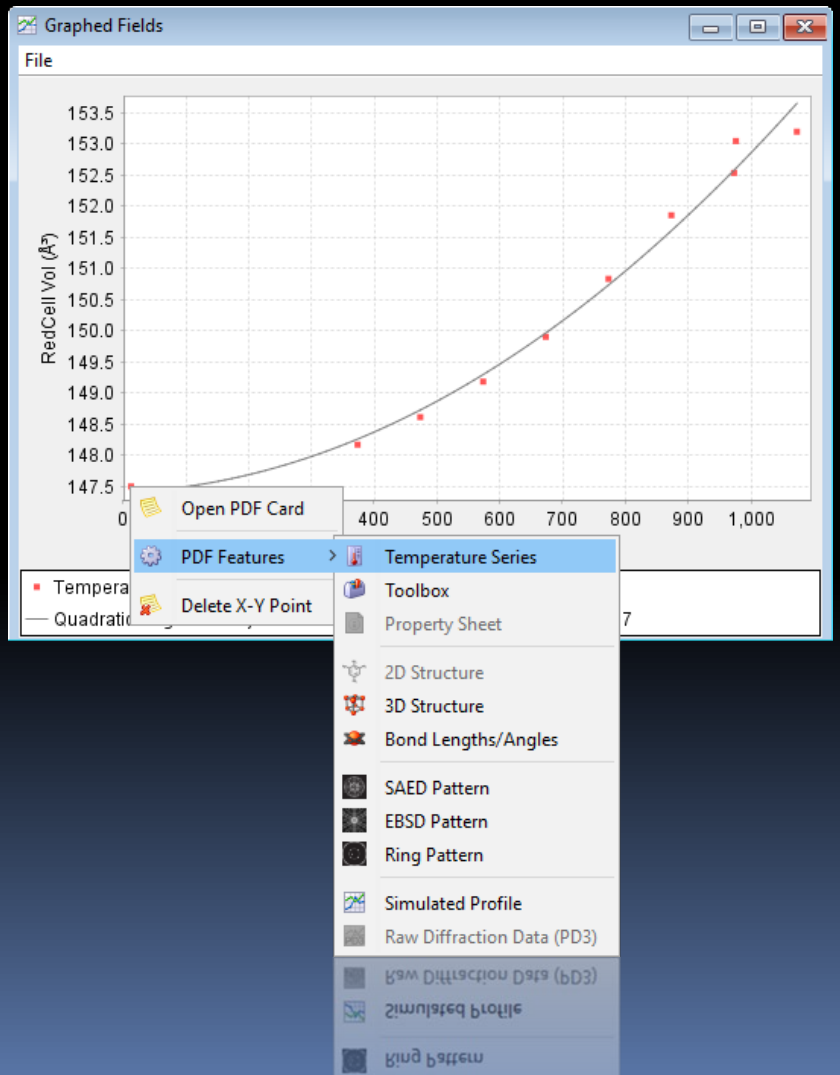
- New Bioactive subclasses
  - Depressants
  - Pesticides & Antimicrobials
  - Stimulants
- New Mineral subclass
  - Clays
- IMA number search

Custom PDF Sets



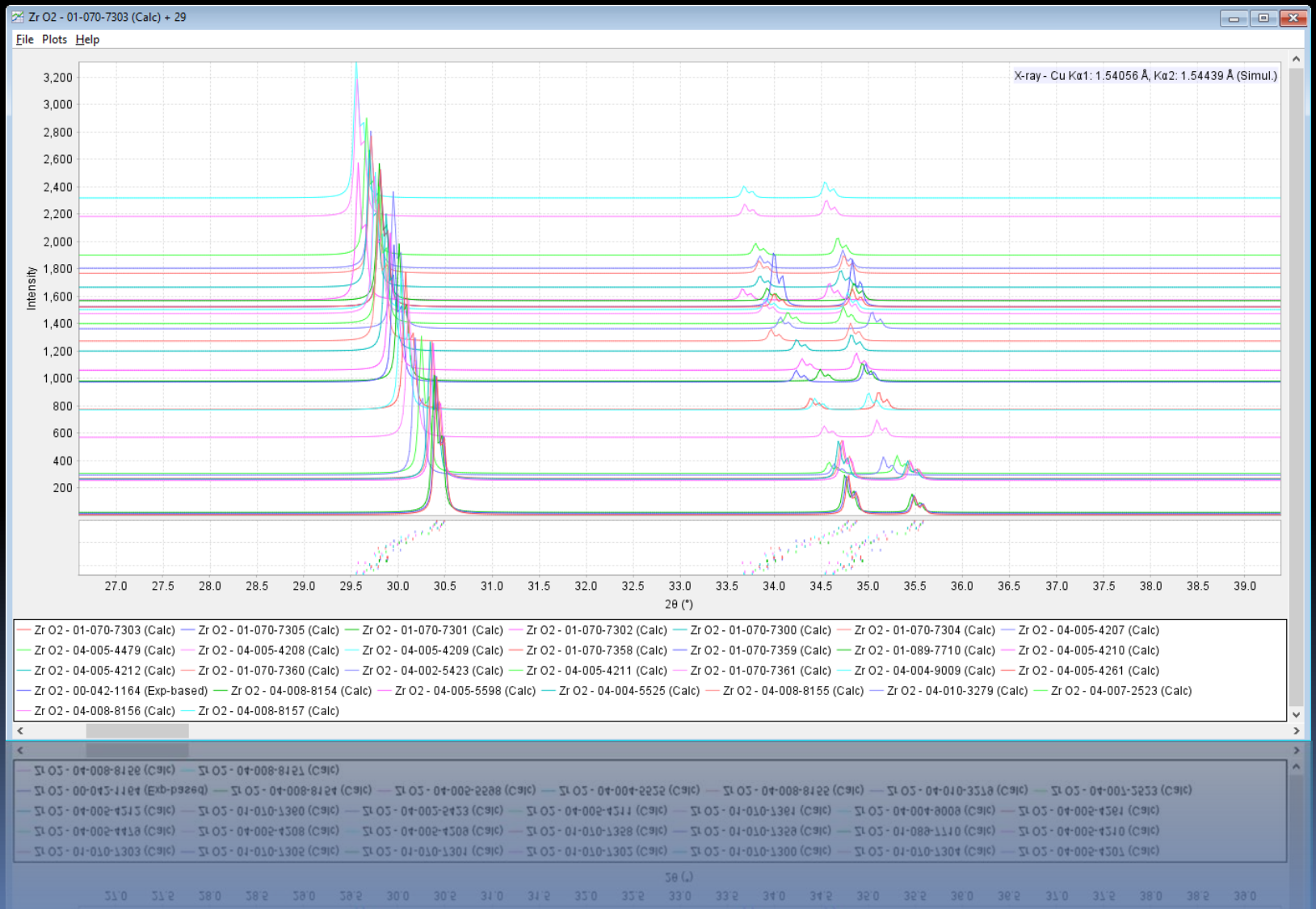
- User-defined sets of PDF entries
- Right-click Custom PDF Sets in search form to **delete** or **rename**

Data Mining Graphs

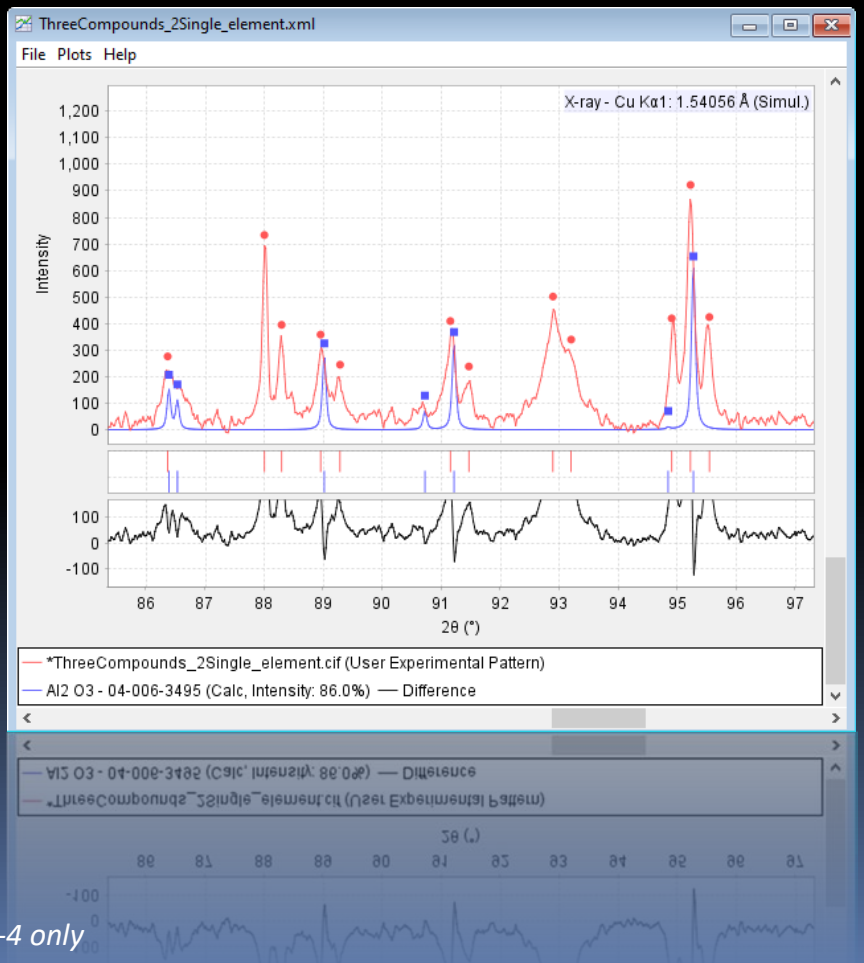


- Each x-y point represents a PDF entry
- Right-click x-y points for tool/simulations
  - 3D structures
  - Ring patterns
  - Etc…
- Manually **delete** outliers

Temperature Series Intensity Offsets



Diffraction Pattern Simulations



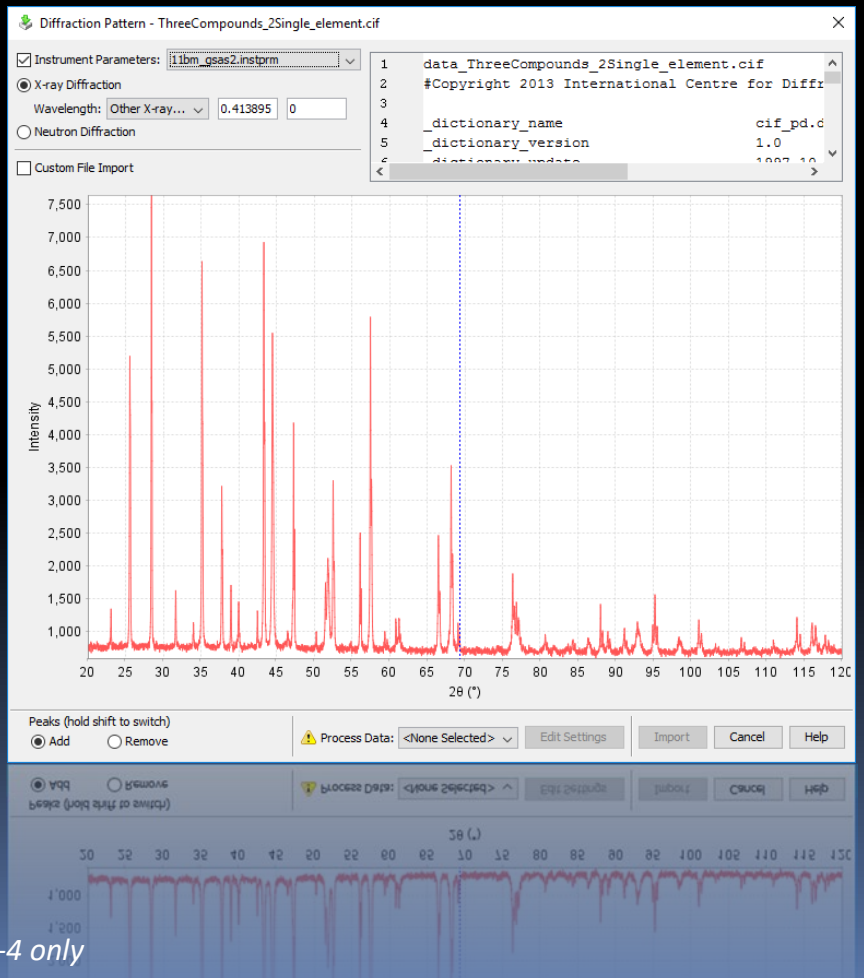
- Show peak symbols at **top** of peaks
  - Allows phase distinction in B&W publications
- Line Width and Font settings **saved** between program sessions
- Tooltips in graph legend display **geometry** and **profile function** settings*

*PDF-4 only

Crystallite Size Slider for Estimation*

*PDF-4 only

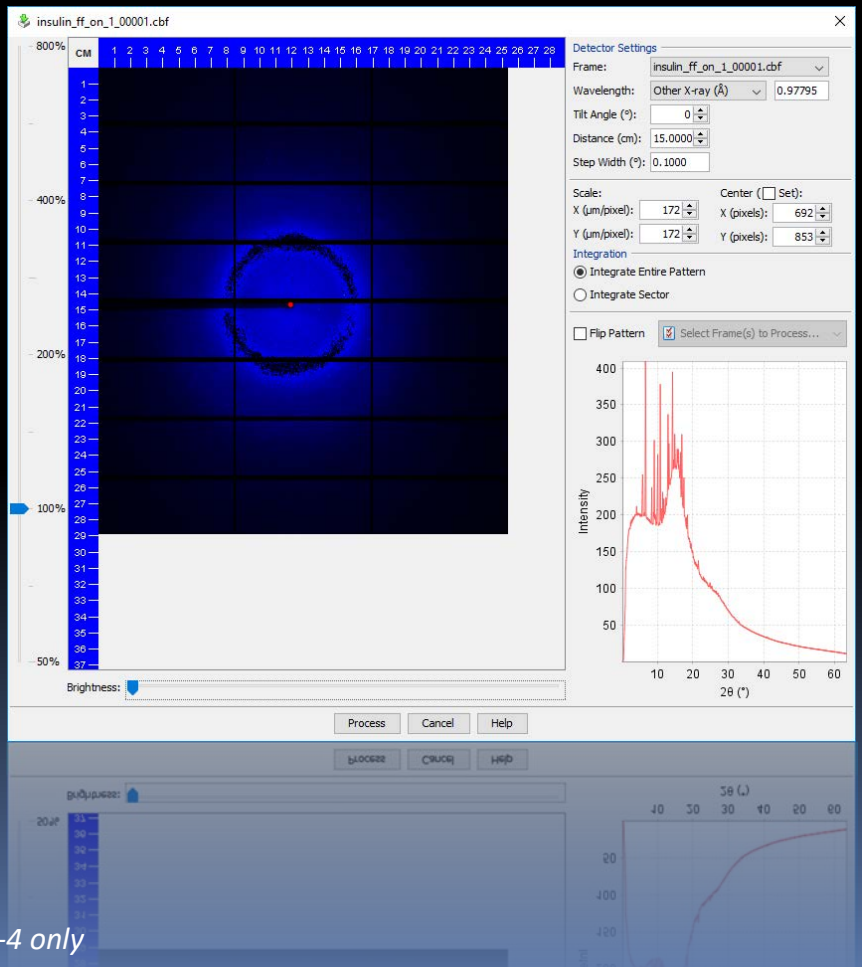
Importing Diffraction Data



- When importing experimental data, choose instrument parameters from **synchrotron** and **neutron** beamlines (FullProf, GSAS, GSAS-II)*
  - Necessary for accurate diffraction pattern simulations
- User-defined **Kα1/Kα2** for removing the Kα2 profile
- User-defined **2θ zero correction**
- User-defined **stop line** for importing custom experimental data files
  - **Good for multi-bank data!**

*PDF-4 only

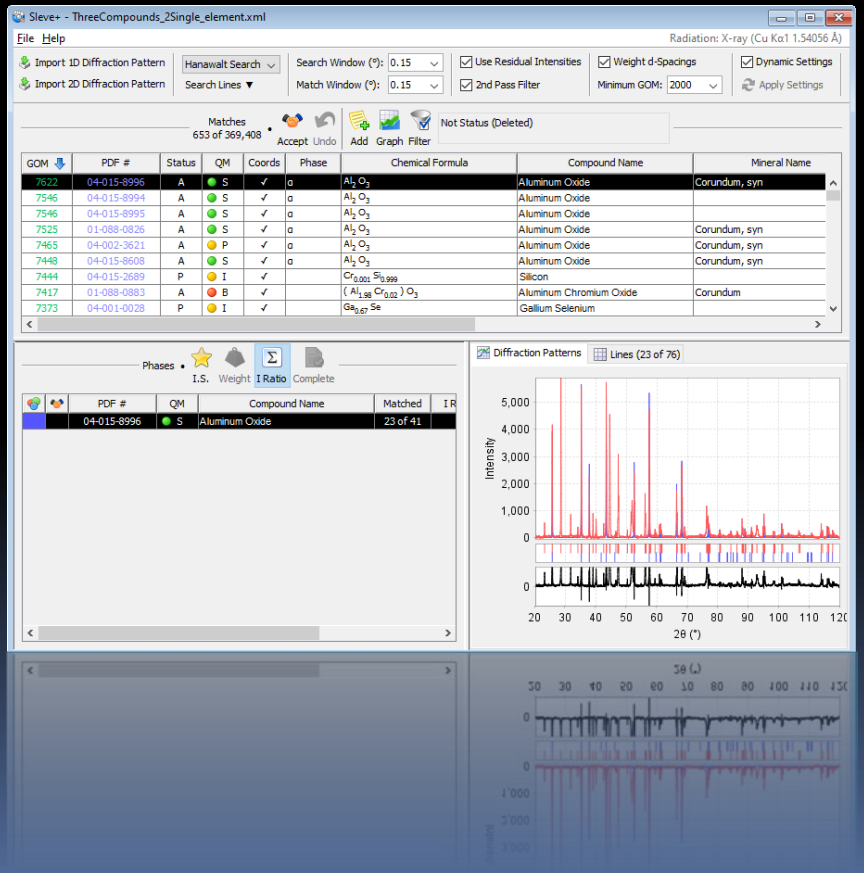
Importing Diffraction Data



- DECTRIS 2D diffraction patterns (*.cbf)*
  - PILATUS detector
  - Array of detector modules in a single image
- 2D diffraction TIFF images*
  - Popular format for 2D diffraction patterns

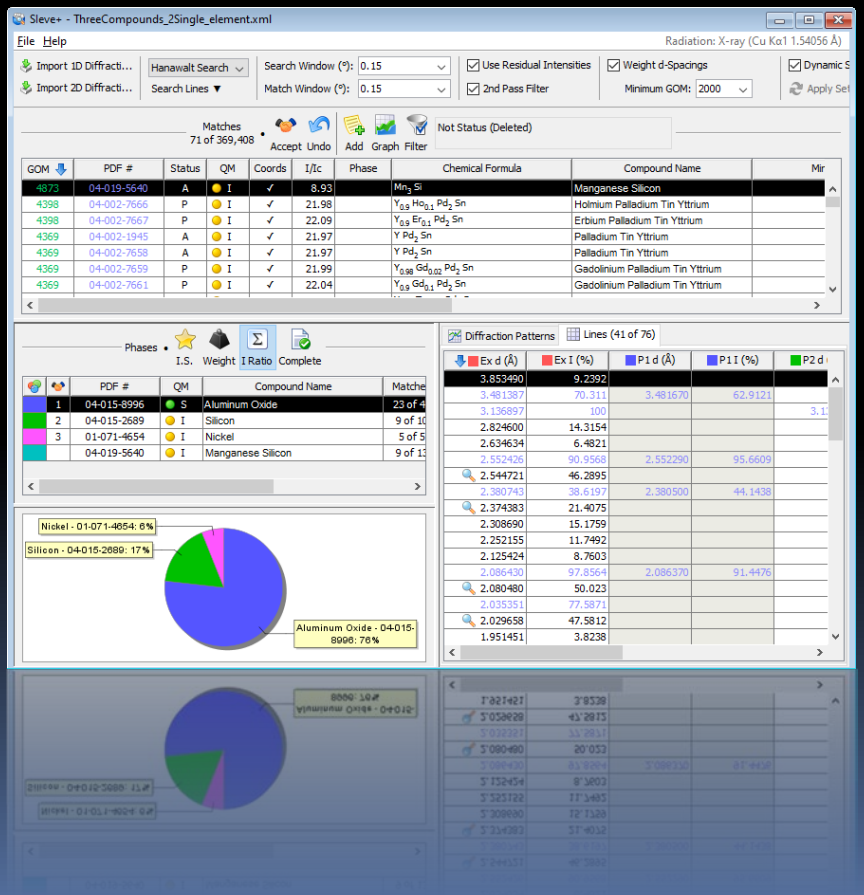
*PDF-4 only

Sleve/Sleve+ Dynamic Settings



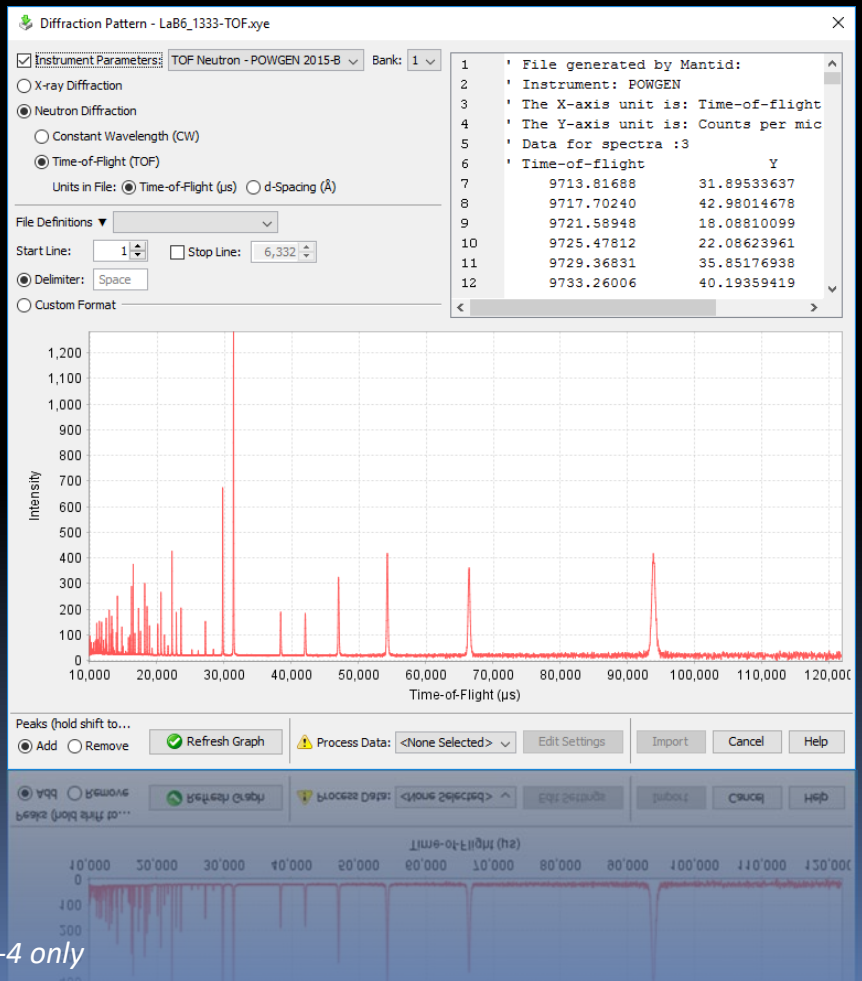
- Search algorithm
- Search window
- Match window
- Minimum GOM

Sleve/Sleve+ Features



- Current search lines highlighted in Lines table
- Semi-quantitative analysis pie chart always visible*
- Customize matches table using 80+ display fields
- Add/remove search peaks directly on graph
- NIST SRM's for correction algorithms (2θ shift, transparency, displacement)
  - NIST SRM 640 (Si)
  - NIST SRM 660 (LaB_6)
  - NIST SRM 675 (Mica)
  - NIST SRM 676 (Al_2O_3)

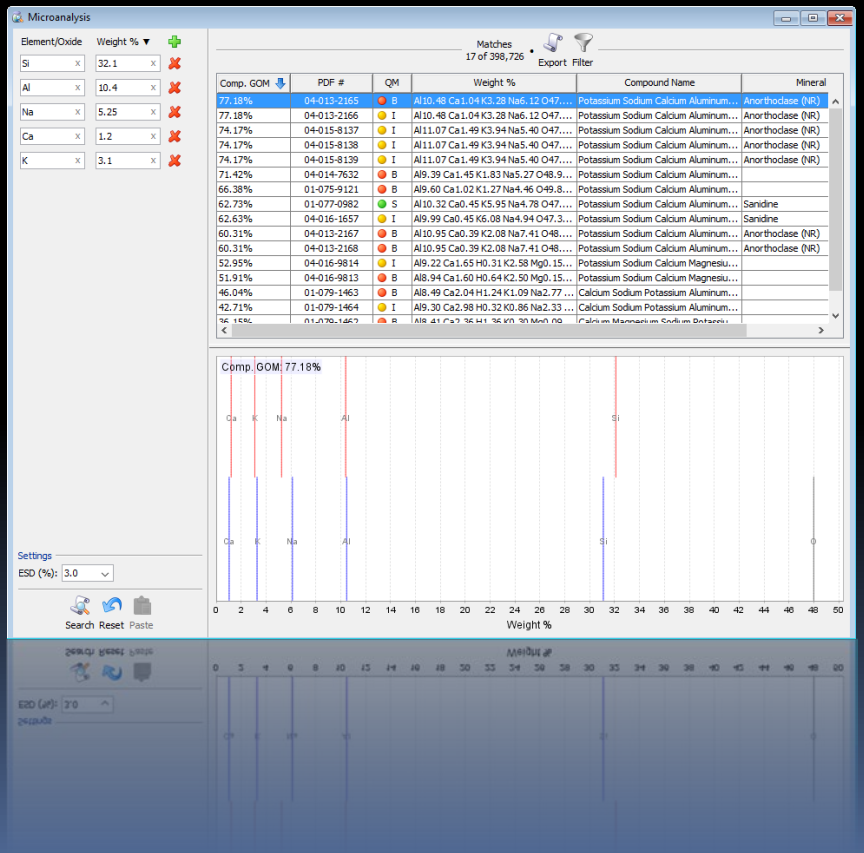
Importing Time-of-Flight (TOF) Neutron Data*



- TOF CIF's
- TOF GSAS files
  - Multi-bank files
- Custom TOF files
- Units in TOF or d-spacing
- Remove background
- Smoothing
- Peak finding

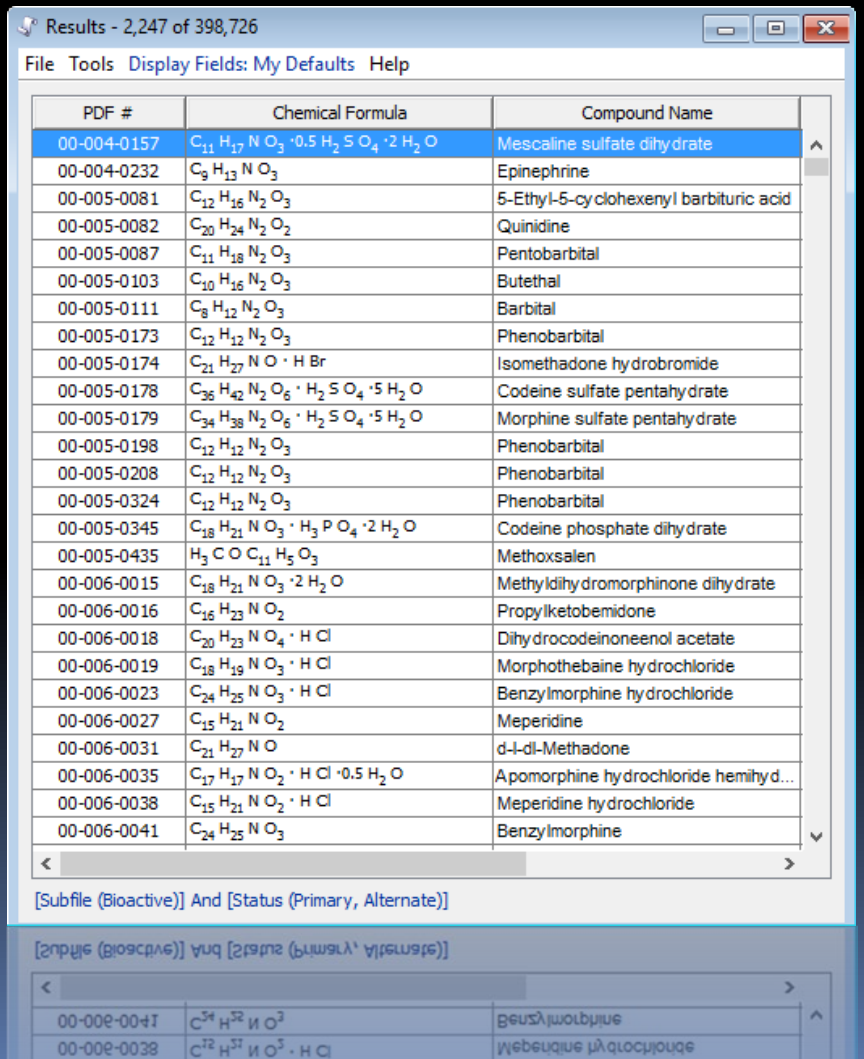
*PDF-4 only

Micro-XRF / Microprobe Analysis Search



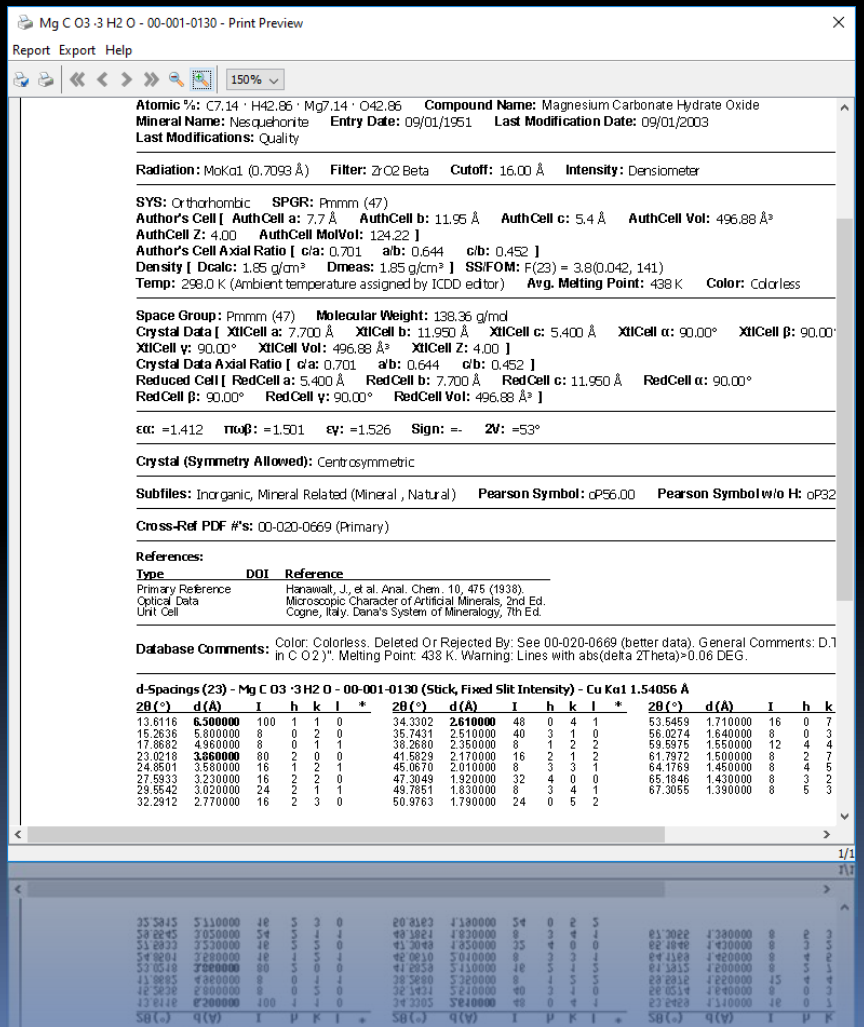
- "Souped-up" composition search with Goodness-of-Match algorithm
- Type or paste composition data from a spreadsheet
  - Elements or oxides
  - Weight % or atomic %
- Ranks best patterns based on composition matching algorithm
- Dynamic composition "stick graph"

User Interface



- Formulas use **subscripts** and **superscripts** for proper notation and readability
  - Chemical Formula
  - Empirical Formula
  - Structural Formula

Printing Reports



- Page setups are **saved** for each report type
  - PDF Card
  - Diffraction Patterns
  - Sleve+
  - etc…
- Page setups are **saved** between program sessions