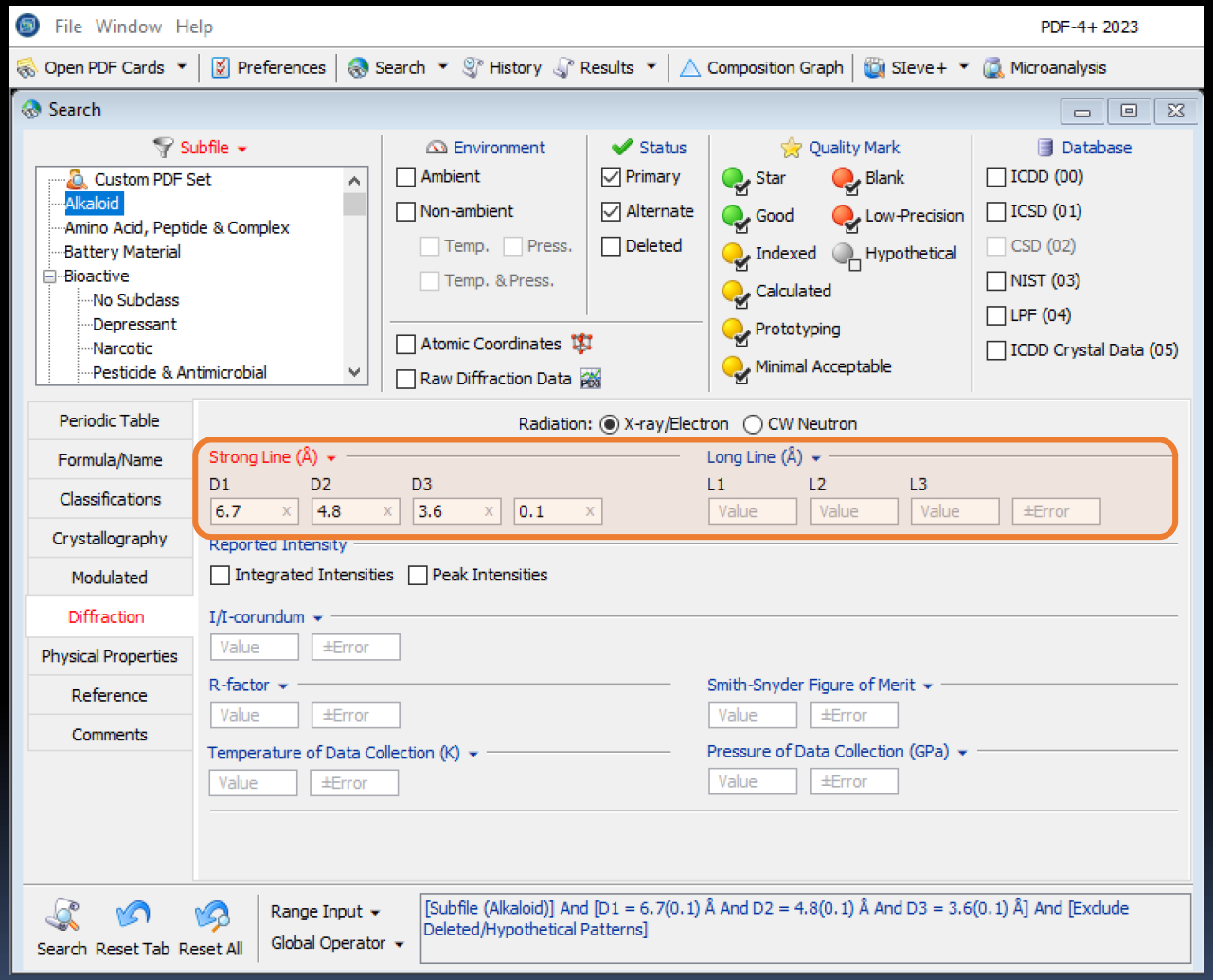
New Features for Release 2023

New Data Mining Features

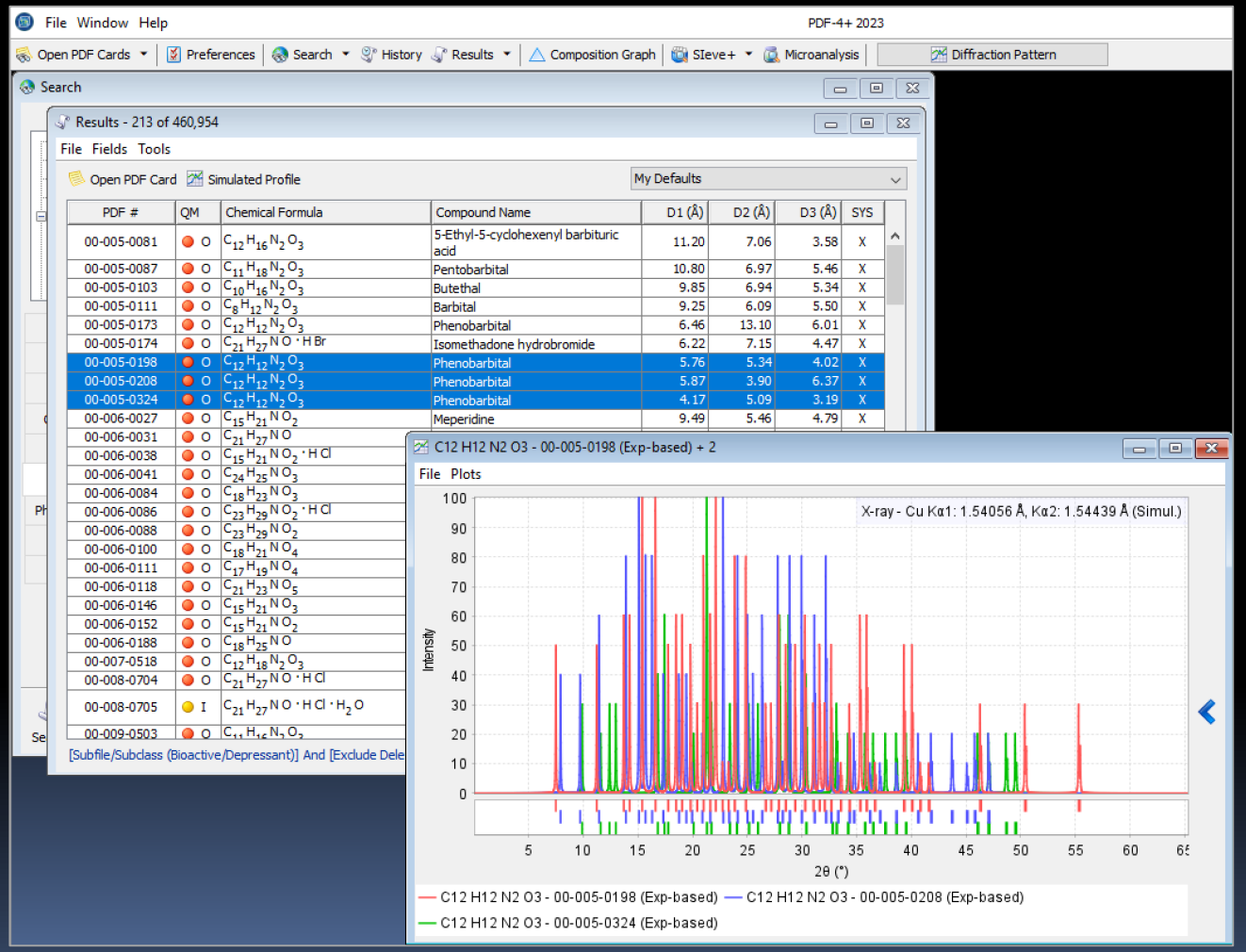
- Metal-Organic Subfile – Phases containing organic moiety with metal(s) belonging to at least one of the following categories
  - Alkali Metals
  - Alkaline Earth Metals
  - Transition Metals
  - Lanthanides
  - Actinides
  - Other Metals (Al, Ga, Ge, In, Sn, Sb, Tl, Pb, Bi, Po)
- Select periodic table elements by typing element symbols or names
- Strong line and long line searches allow simultaneous input of three different search lines
  - Allow permutation of lines



Strong line search for three different lines simultaneously

New Graphing Features (PDF-4)

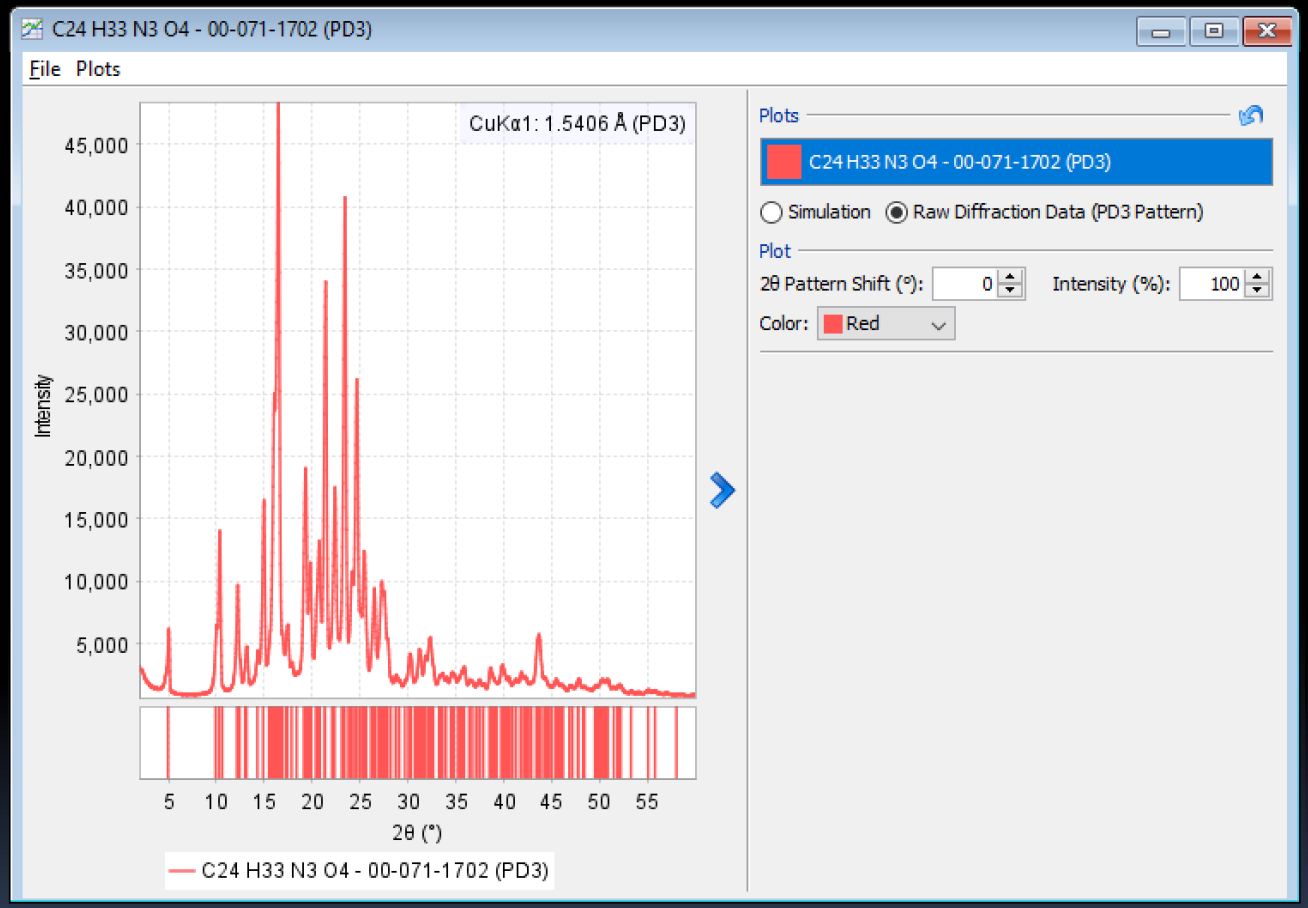
- Drag diffraction pattern files from the File Explorer directly into the program
- Drag PDF entries from any search results table to a diffraction pattern window
  - Multiple entries supported
  - Simulated, raw (PD3), and stick patterns



Three Phenobarbital entries from the search results table were dragged into the diffraction pattern window using the mouse

New Graphing Features

- Quickly switch between simulations and raw patterns using the quick settings pane (in PDF-4)
- Hold SHIFT key to view x-y coordinates of the mouse
- Right-click menu allows user to copy x-y data to system clipboard



PD3 pattern of Ranolazine can be adjusted directly in the quick settings pane

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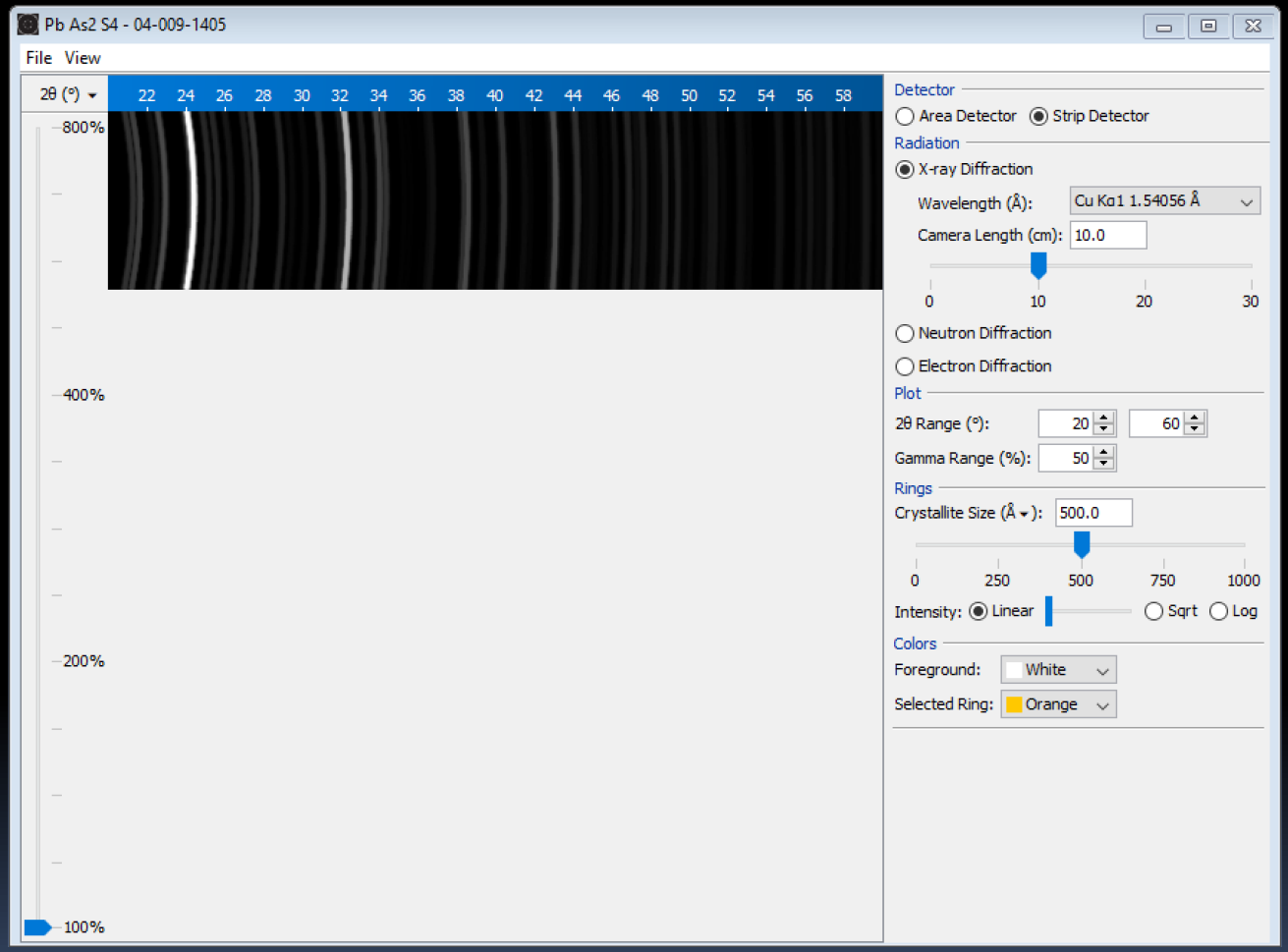
New 2D Ring Pattern Features (PDF-4)

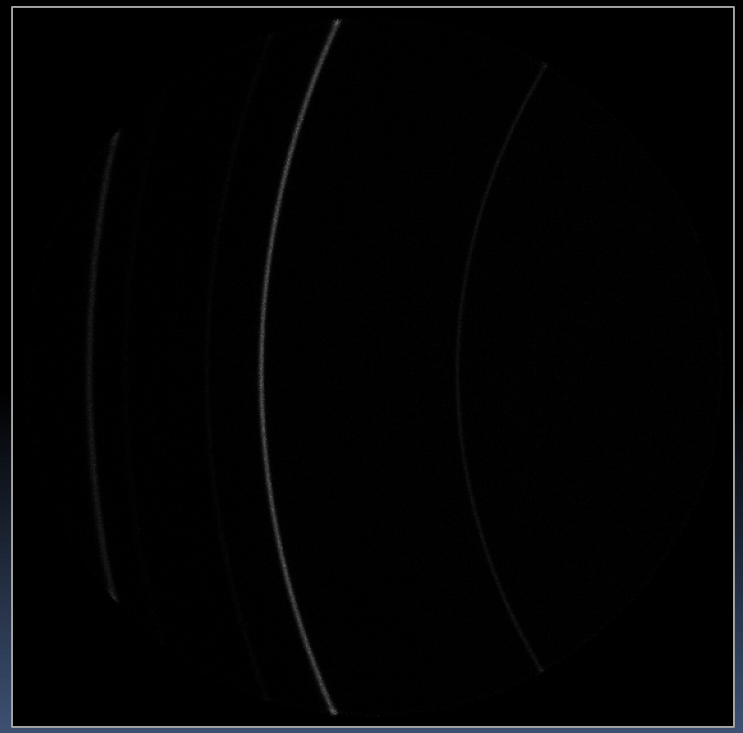
- Strip detector simulations
  - 2θ range setting
  - Gamma range setting
- Display axis in Q space ($Å^{-1}$), d (nm), 1/d ($Å^{-1}$), 1/d (nm^{-1})
- Hold SHIFT key to view 2θ coordinates of the mouse
- Intensity scale settings
  - Linear
  - Square root
  - Logarithmic
- Highlight rings using the mouse
- Optimized drawing routines for faster performance
- Enhance imported 2D images using contrast stretching algorithm



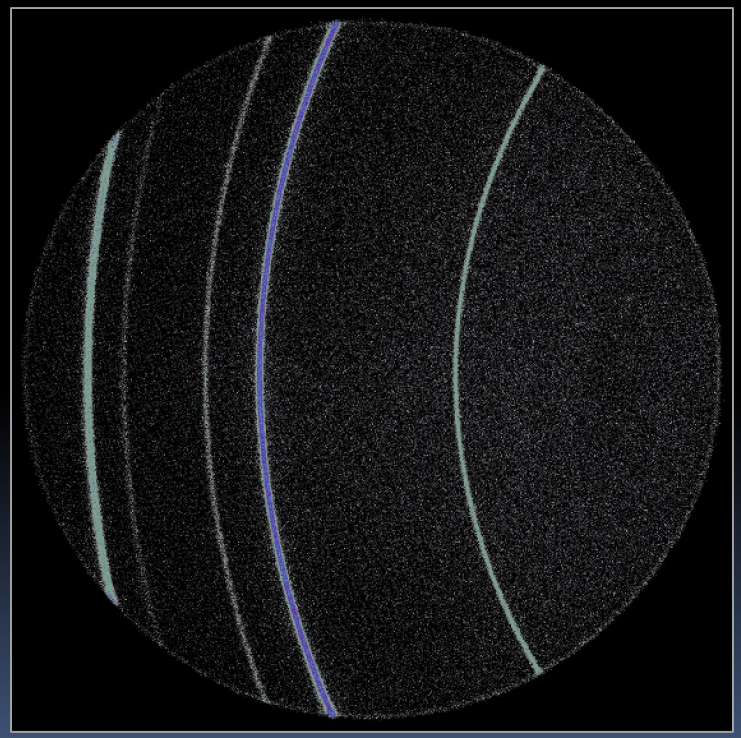
Strip detector simulation of Lead Arsenic Sulfide

Image Contrast Setting (PDF-4 & Sleve+)

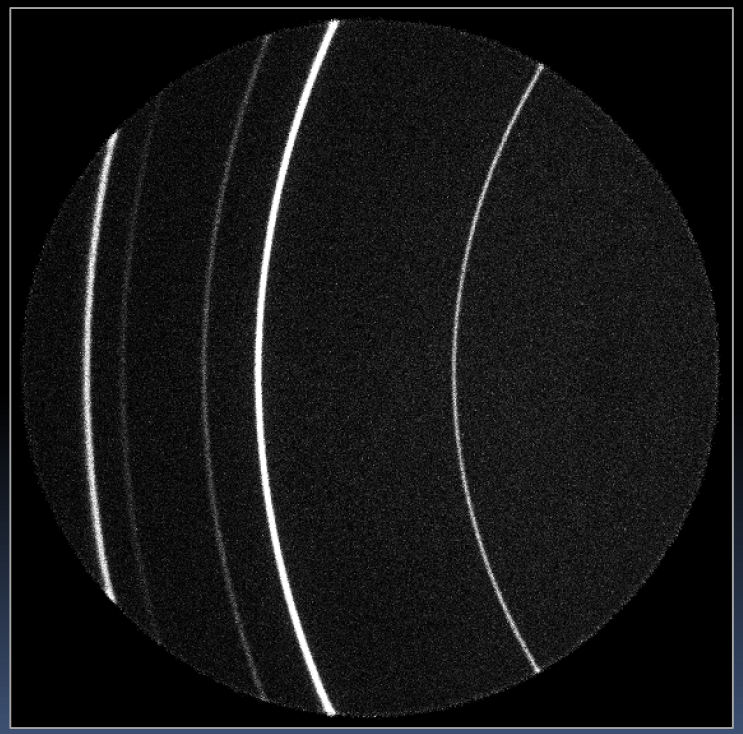
No Contrast



Enhanced Contrast (old)

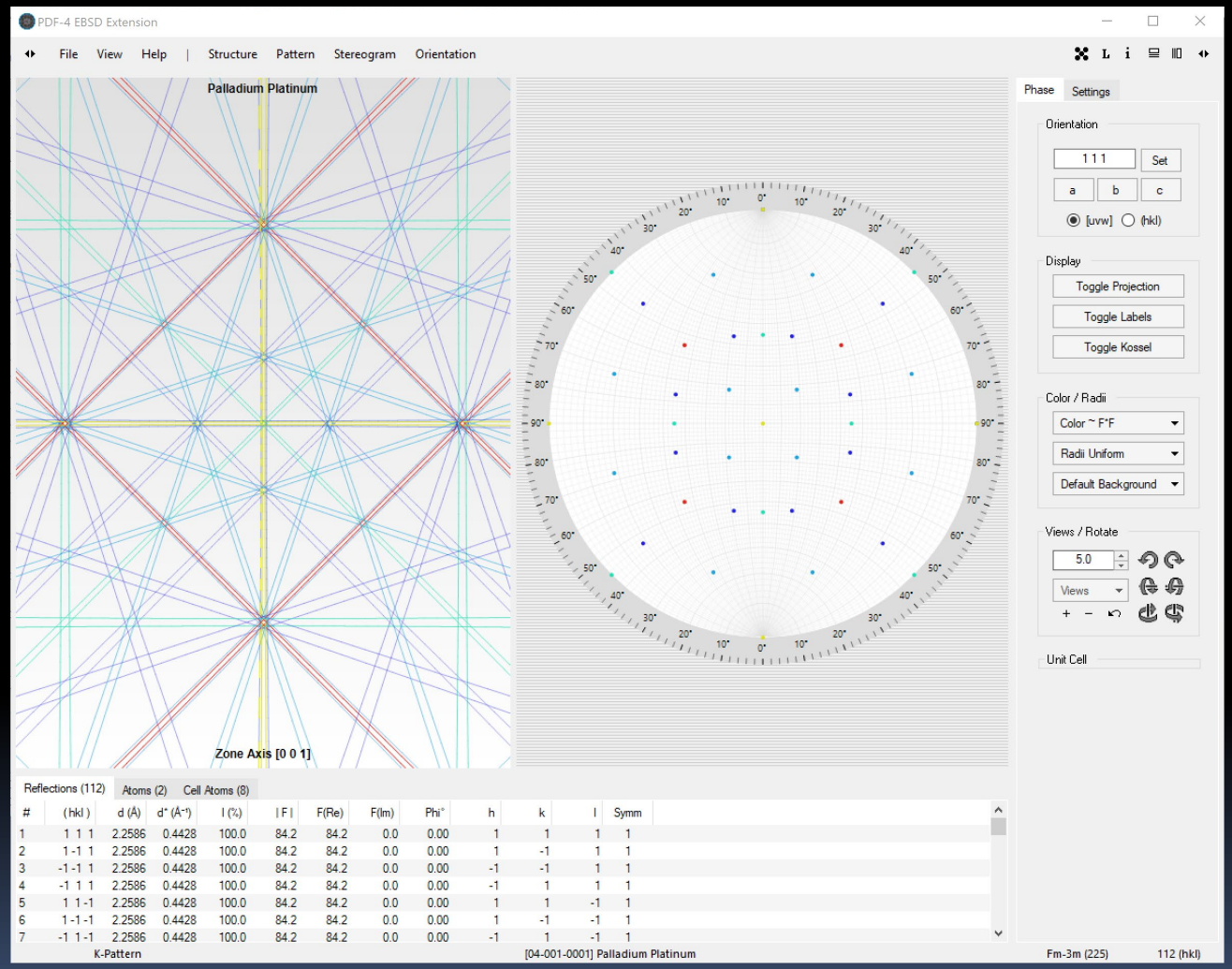


Enhanced Contrast (new)



EBSD Extension (PDF-4)

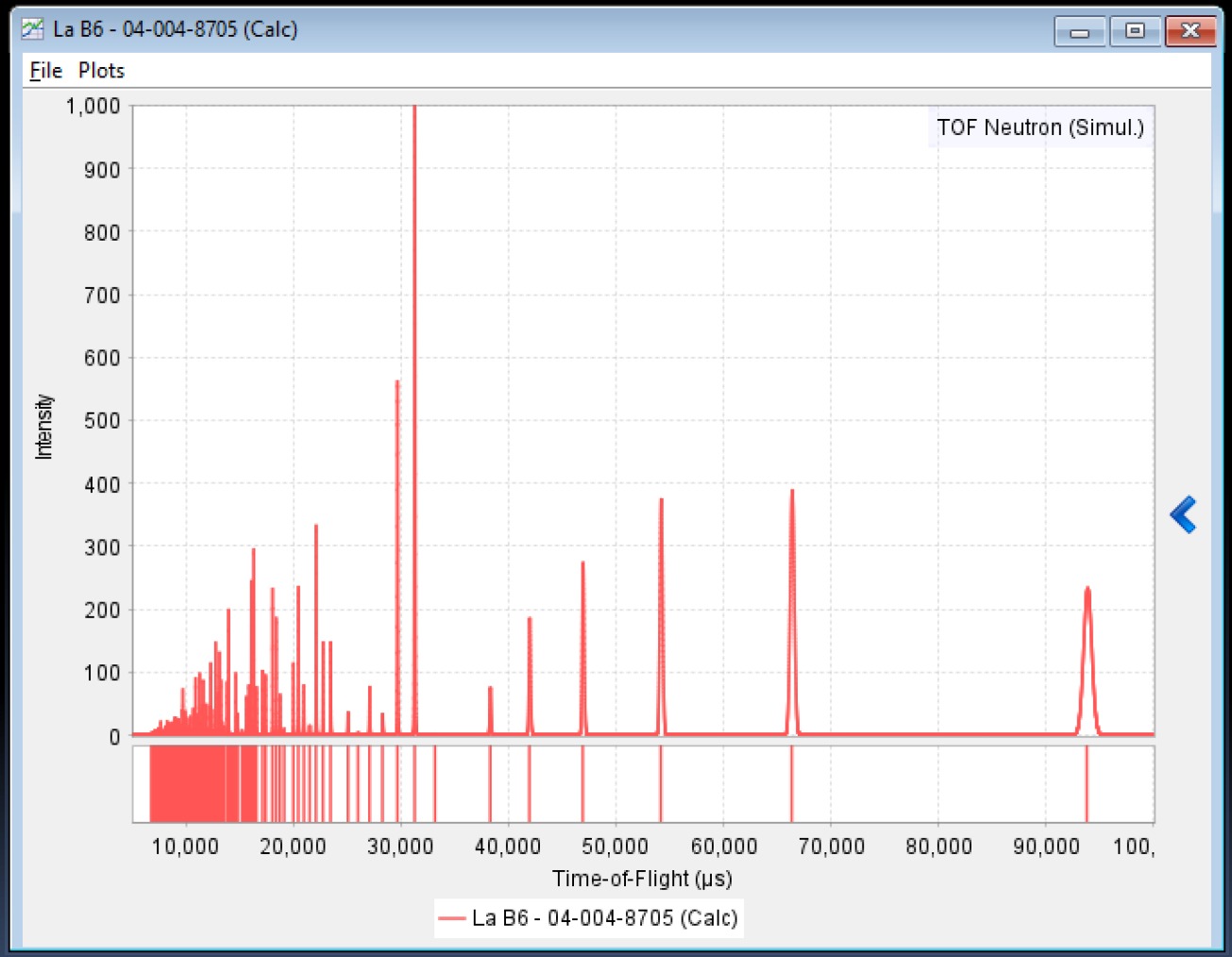
- The EBSD (electron backscatter diffraction) extension is designed to plot K-patterns (Kikuchi & Kossel patterns)
- Toggle between gnomonic projection and stereographic projection
- For Kossel patterns, up to three Kα1-wavelengths of elements in the chemical formula are used
- Can be accessed on the PDF card window or EBSD window



EBSD extension for Palladium Platinum (04-001-0001)

New Features for Phase ID (SIeve+)

- Import GNR *.esg diffraction patterns
  - Analytical Instruments Group
- Import neutron TOF instrument parameters for GSAS-II files
  - POWGEN cycles 2017-AB – 2022-A



TOF simulation of LaB6 using GSAS-II instrument parameters (POWGEN cycle 2022-A)

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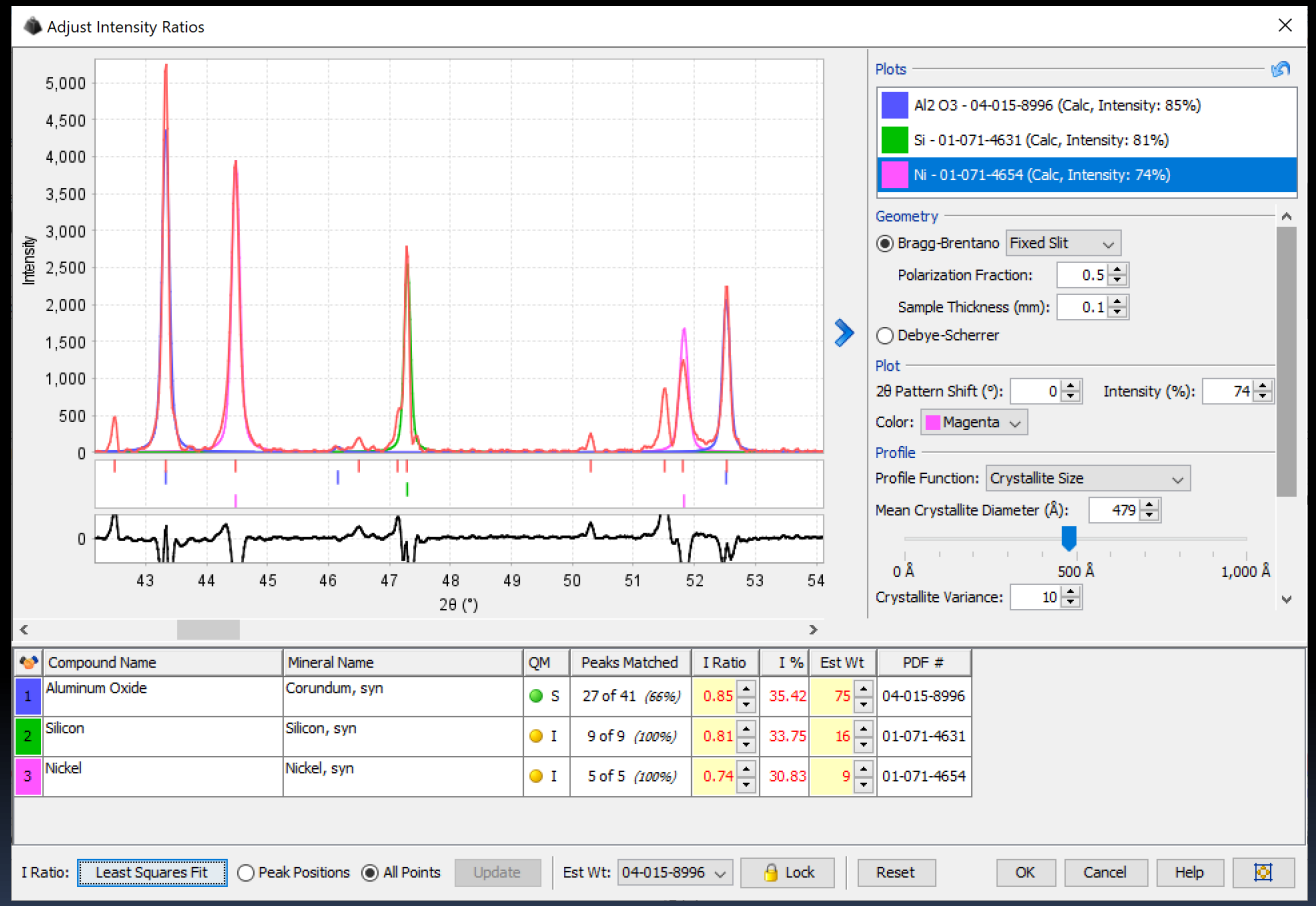
New Features for Phase ID (SIeve+)

- Supports new internal standard NIST SRM 640f
- Least squares RIR quantitative analysis can use all points for more accurate fitting of data
- Matches filter displays the current search description



Least squares RIR optimization of quantitative analysis of three phase mixture

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