New Features for Release 2022

New Topology Searches

Topology Volume Search

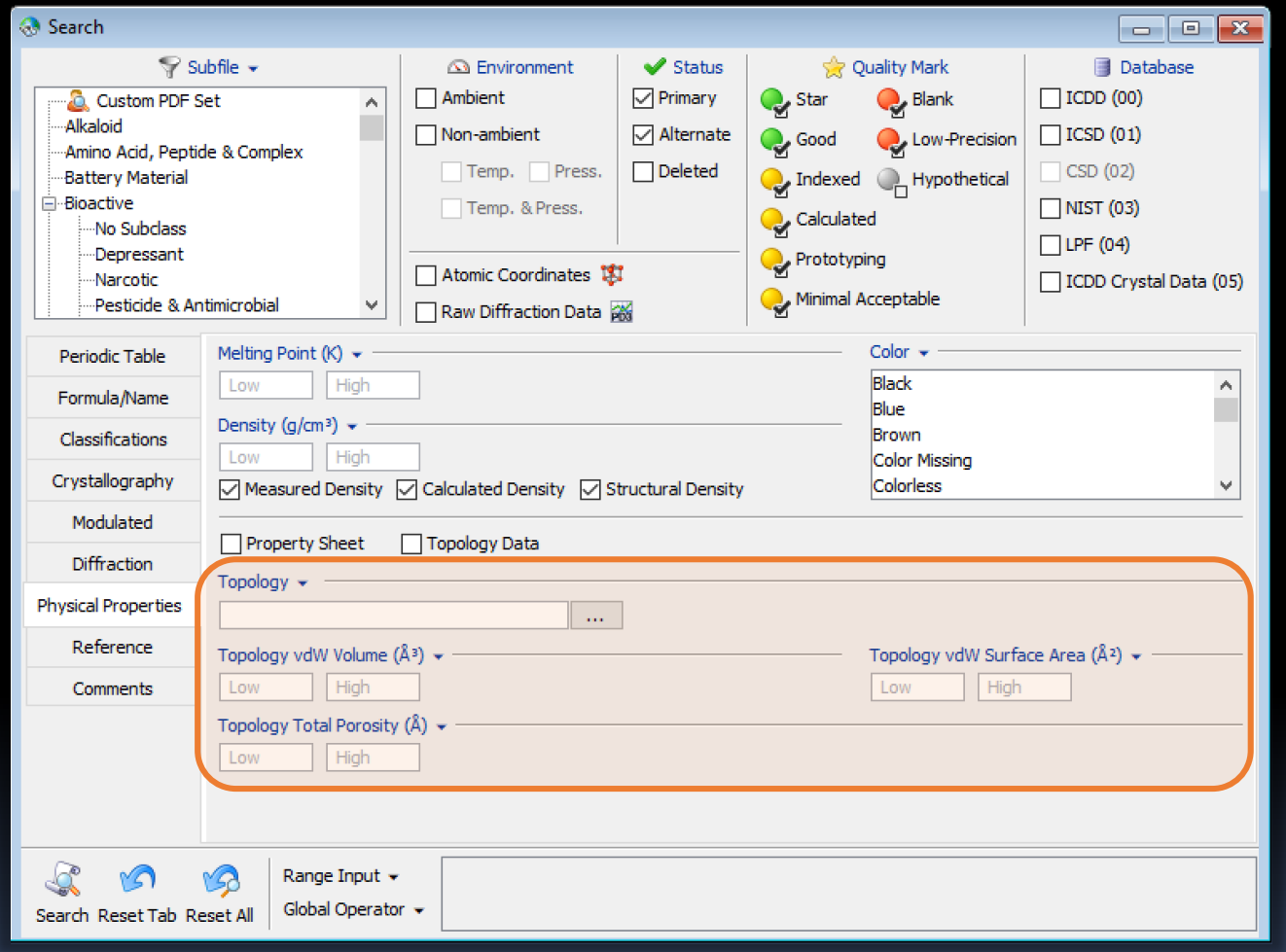
- The volume (V_{vdw}) of space confined by van der Waals surface of atoms in the unit cell and boundaries of unit cell

Surface Area Search

- The area (S_{vdw}) of van der Waals surface of atoms in the unit cell

Total Porosity Search

- The percent of empty space in a structure



New topology data mining searches located in the Physical Properties tab.

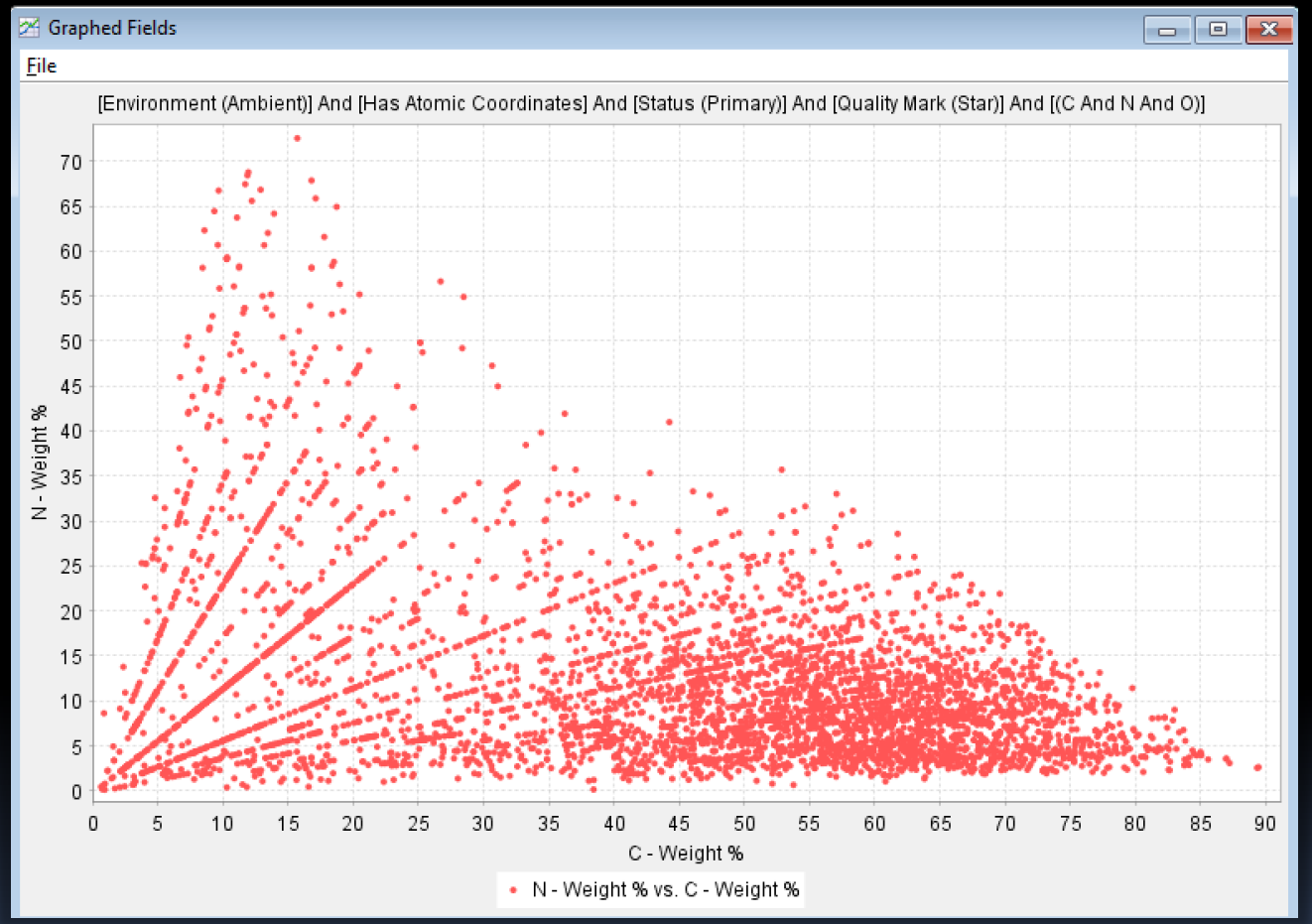
New Features for User-Created Graphs

Weight % and atomic % values can be graphed against themselves

Customize the size of graph data points for publication use

- Small points
- Medium points
- Large points

Export regression coefficients to spreadsheet programs



Graph of wt% of carbon vs wt% of nitrogen for PDF entries containing carbon, nitrogen, and oxygen.

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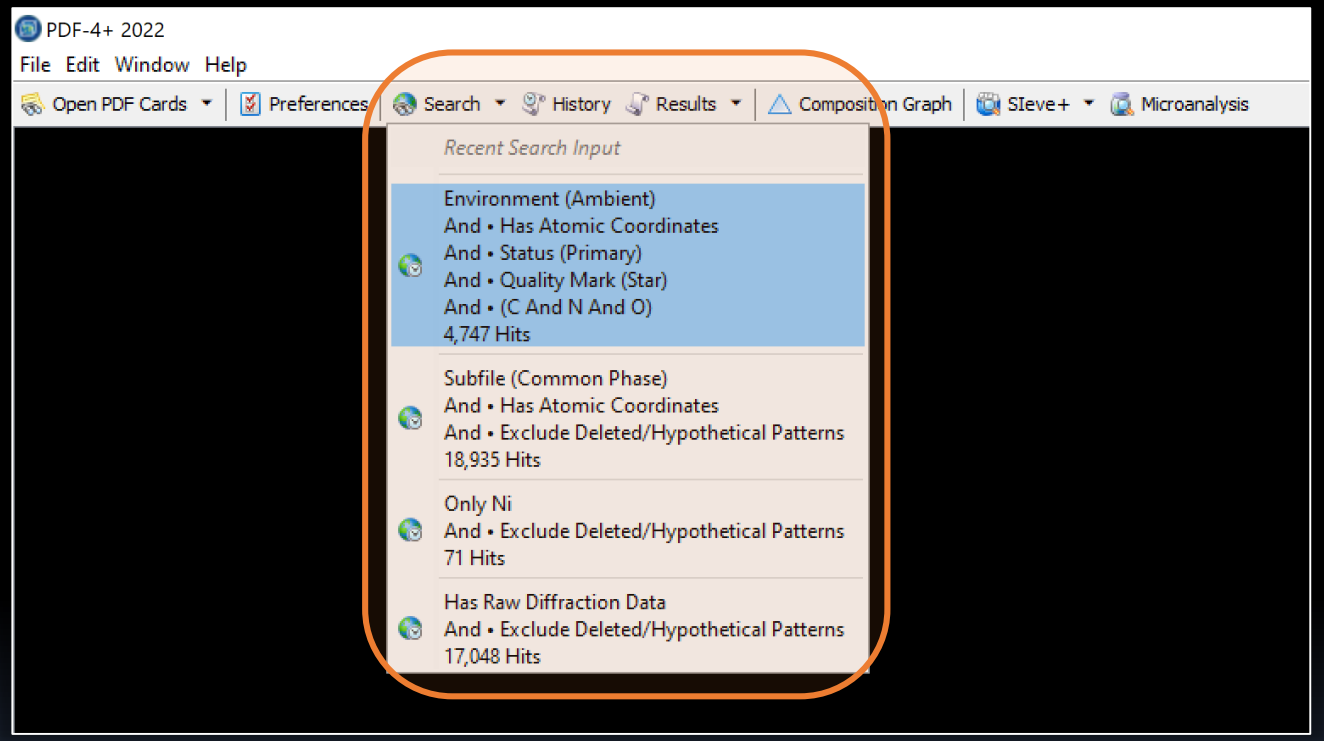
Drop-Down Menu of Recent Search Input

Easily re-populate search input from any past search using new drop-down menu

Save time by no longer having to re-enter search input

Drop-down menu contains full search description and number of hits



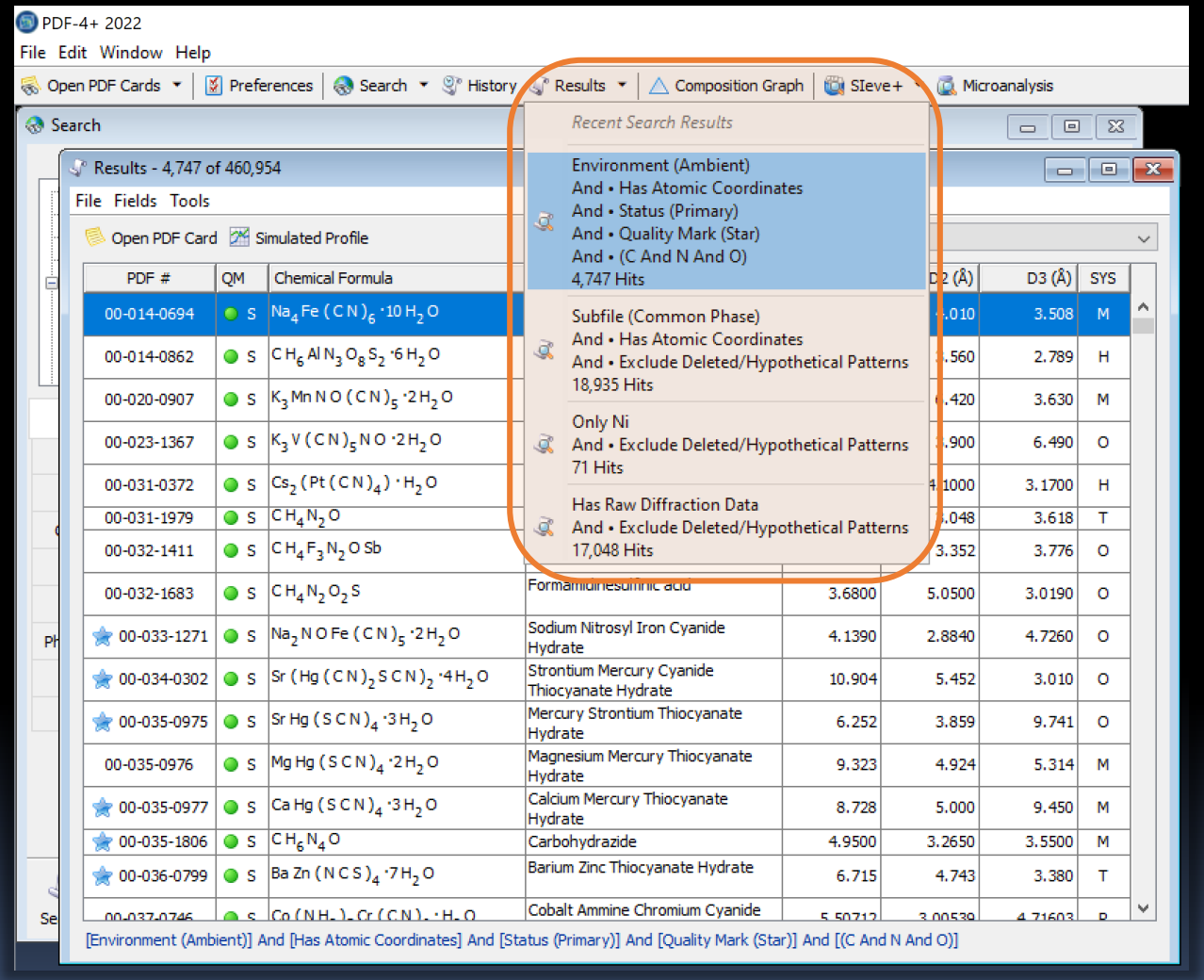
Drop-down menu of recent data mining search input.

Drop-Down Menu of Recent Search Results

Quickly toggle between previous search results using new drop-down menu

Drop-down menu contains full search description and number of hits

All searches are saved/restored using XML files



Drop-down menu of recent data mining searches.

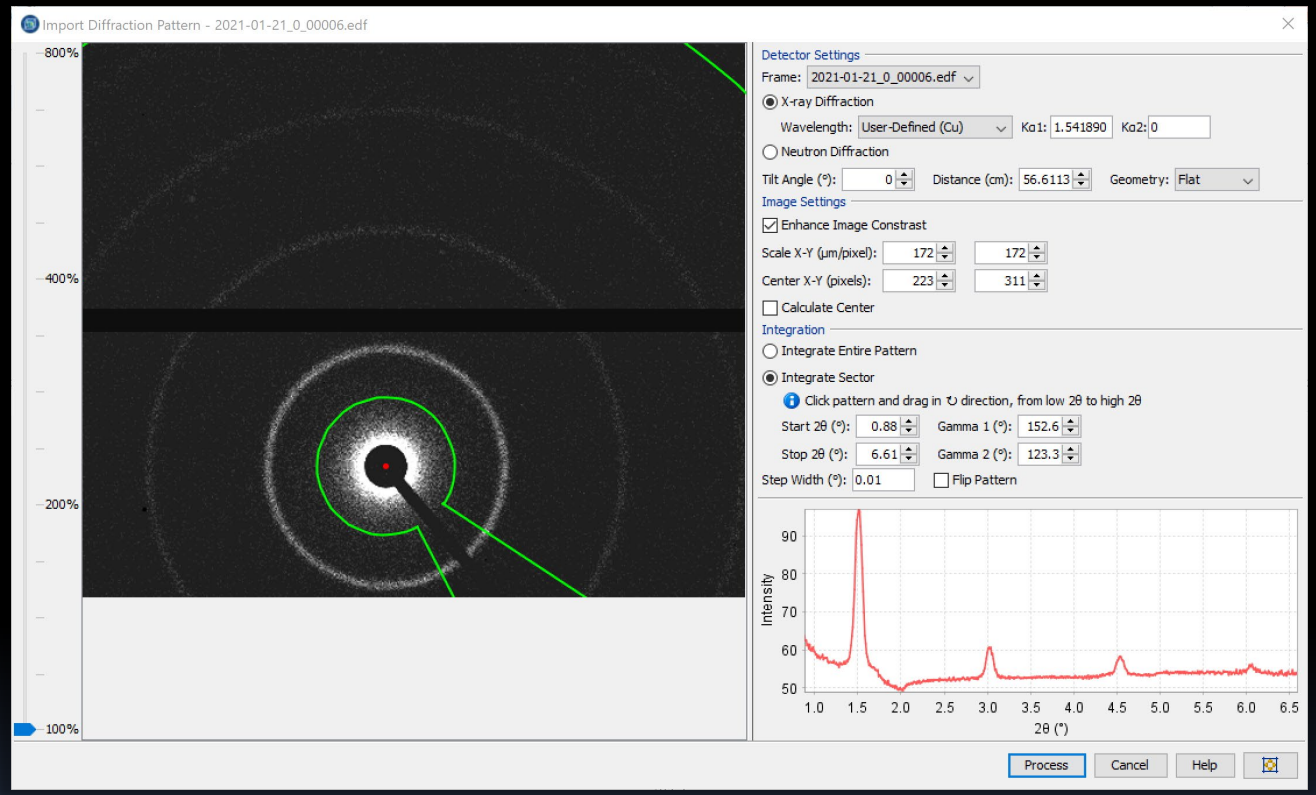
New Features for Importing Diffraction Data

New supported file types

- *.txl files (1D diffraction)
- ESRF *.edf files (2D diffraction)

Enhance the contrast of imported 2D images (*.jpg, *.png, *.tiff)

Optimized importing files over a network



Integration of an ESRF 2D diffraction pattern of silver behenate for phase ID.

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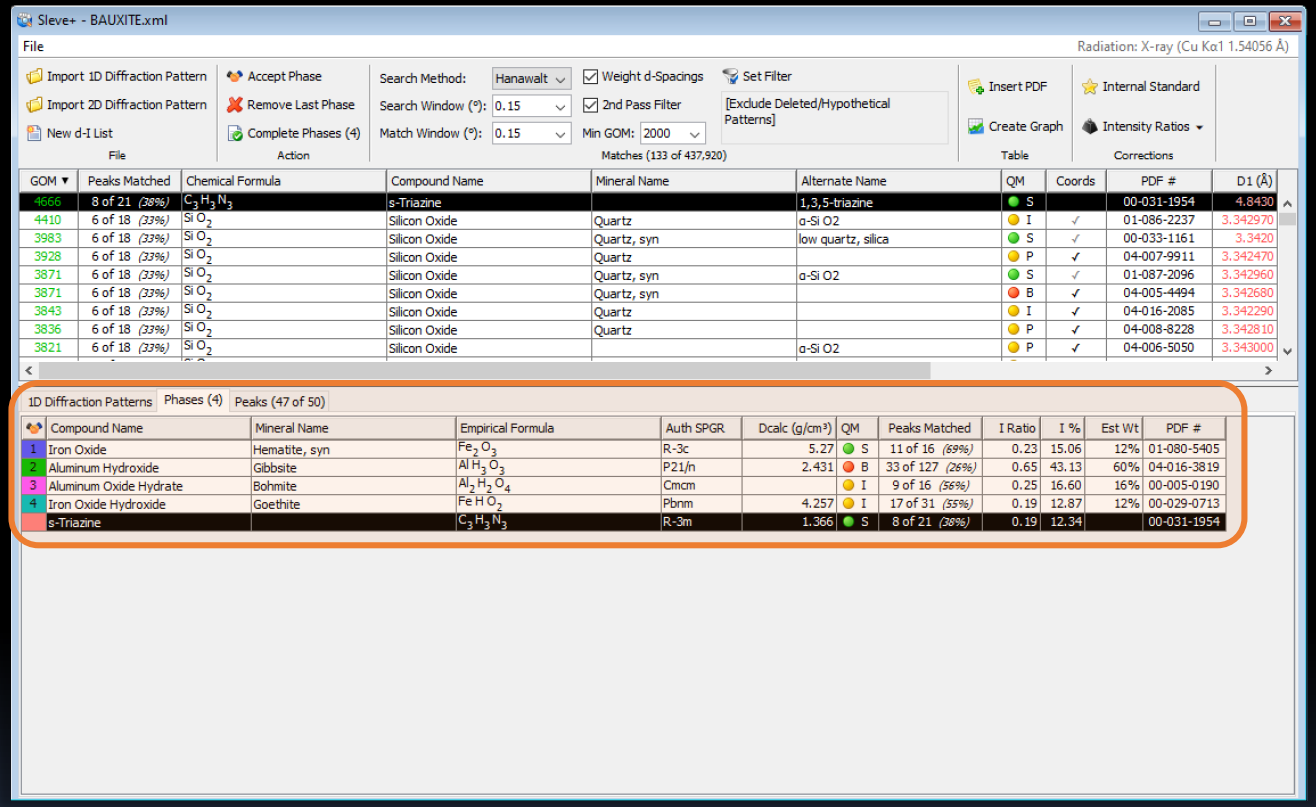
New Features for Phase ID (SIeve+)

Customize display fields for the phases table

- Access to 85+ display fields
- Display fields are remembered between program sessions

Prefer mineral name in graph legend



The phases table in SIeve+ with user-defined display fields (empirical formula, space group, and calculated density).

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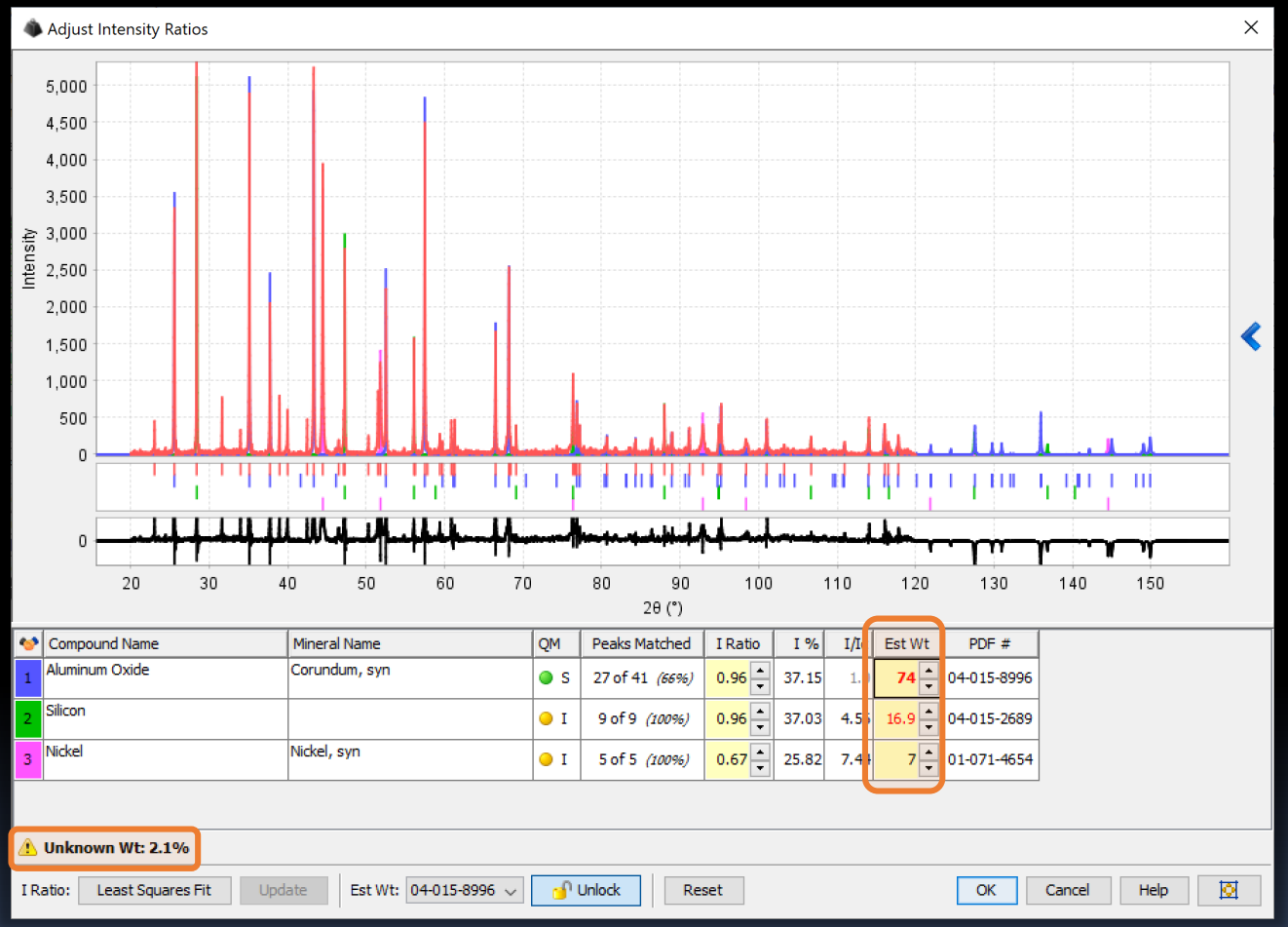
New Features for RIR Quantitative Analysis

Lock the wt% of a specific phase (as an internal standard) for RIR analysis

- Using standard addition or XRF data
- Unknown/amorphous wt% will be calculated and displayed

User-modified values are highlighted in red



The wt% of corundum is designated as an internal standard using XRF data for RIR quantitative analysis.

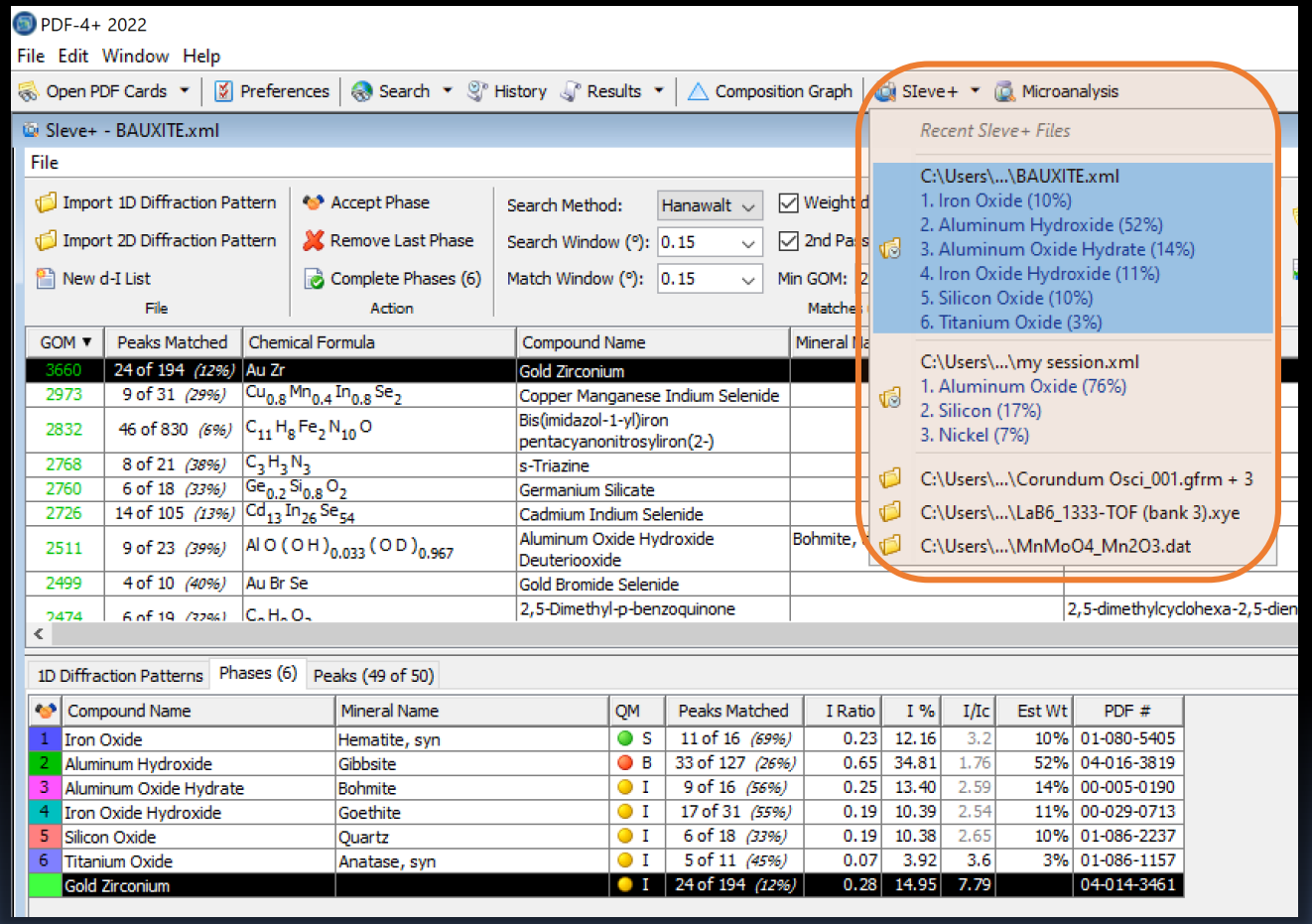
New Features for Phase ID (SIeve+)

Easily open previous SIeve+ session files and imported data files using new drop-down menu

Drop-down menu displays a preview of the accepted phases and their wt%

All SIeve+ sessions are supported

- X-ray diffraction analysis
- Neutron diffraction analysis
  - Constant wavelength
  - Time-of-flight
- Electron diffraction analysis
- 1D and 2D diffraction patterns



Drop-down menu of all recent SIeve+ session files and imported data files.

New System-Wide Features

- Improved user interface for small screens
  - Option to show smaller toolbar
  - Option to hide program taskbar
- 64-bit support
  - Performance increase for multi-threading operations

	32-bit	64-bit
Similarity indexes (928 patterns)	30s	11s
Similarity indexes (2,853 patterns)	1m 50s	51s
2D integration of one Rigaku file	13s	9s
2D integration of four Bruker files	16s	12s