



New Features for Release 2025

Autocomplete Name Search

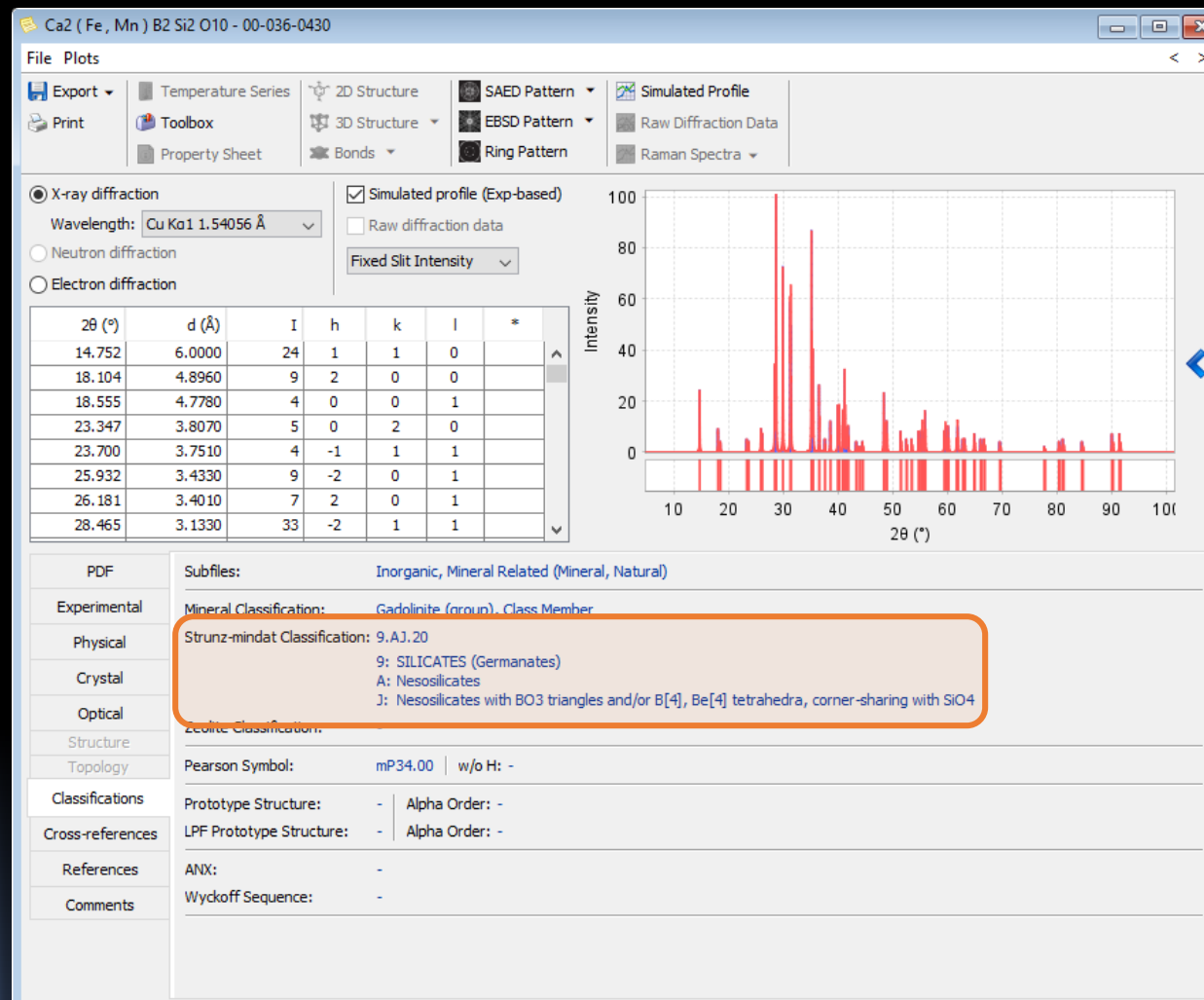
Automatically suggests names based on user input using two methods

1. Uses substring search to suggest similar names
2. Uses machine learning spellcheck library to suggest alternate spellings (if misspelled)

The screenshot displays the ICDD search interface. At the top, there are filters for Subfile, Environment, Status, Quality Mark, and Database. The main search area is divided into several sections: Periodic Table, Formula, Name, 2D Structure, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments. The 'Name' section is active, and a dropdown menu is open, showing suggestions for the input 'quartz'. The suggestions include 'Quartz', 'quartz enfume', 'Quartz glass disk', 'quartz high', 'quartz high, syn', 'quartz HP', 'quartz low', and 'quartz low HP'. The search bar at the bottom contains the query: '[Any Name contains fragments 'quartz'] and [Exclude deleted/hypothetical patterns]'. The 'Hits' section shows a progress bar.

New Mineral Classifications

- Strunz-mindat classifications
 - Search and display field
- IMA mineral symbols
 - Search and display field
- IMA mineral classifications
 - Display field



Dynamic Hit Counts

- Displays search hit counts based on selected criteria
- For data mining searches
- For matches filters
 - Sleeve/Sleeve+
 - Microanalysis
 - Composition graph

The screenshot shows the ICDD Search interface. On the left, there is a 'Subfile' tree with categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'. The 'Bioactive' category is expanded. In the center, there is a 'Periodic Table' with elements B, C, and N highlighted in red. A search filter is applied: '[(B and C and N)] and [Exclude deleted/hypothetical patterns]'. The search results are displayed at the bottom right, showing a hit count of 1,128.

Search

Subfile

Environment

Status

Quality Mark

Database

Periodic Table

Formula/Name

2D Structure

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Boolean

And

Or

Yes/No/Maybe

Only

Just

Composition list

Not

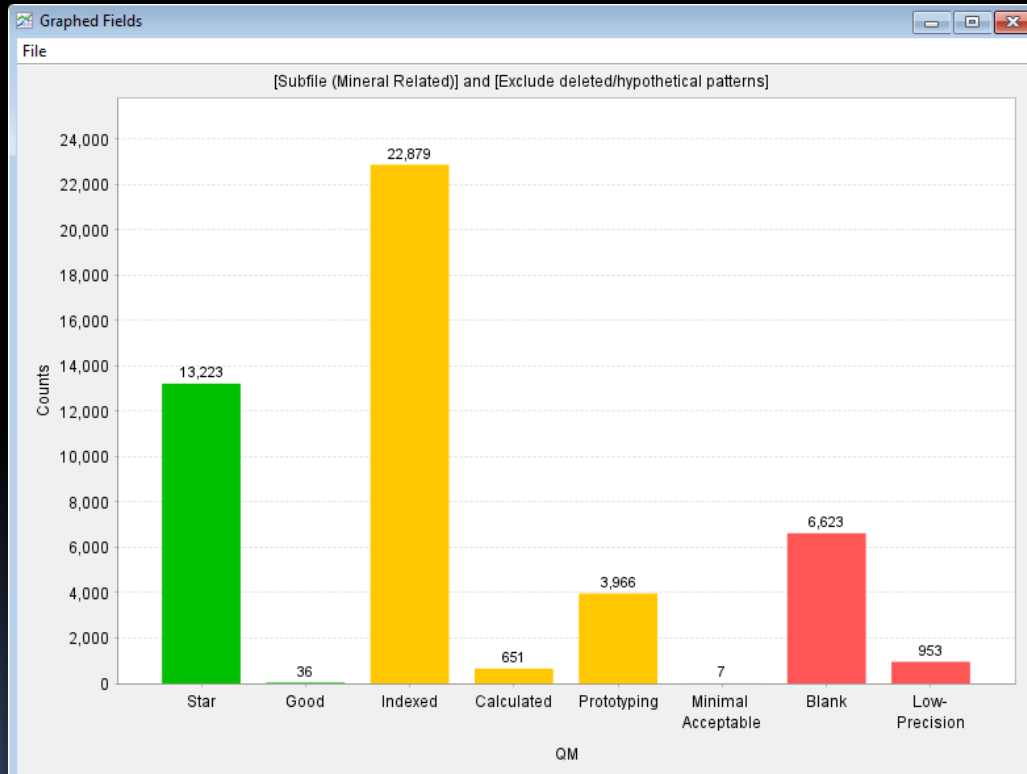
And

[(B and C and N)] and [Exclude deleted/hypothetical patterns]

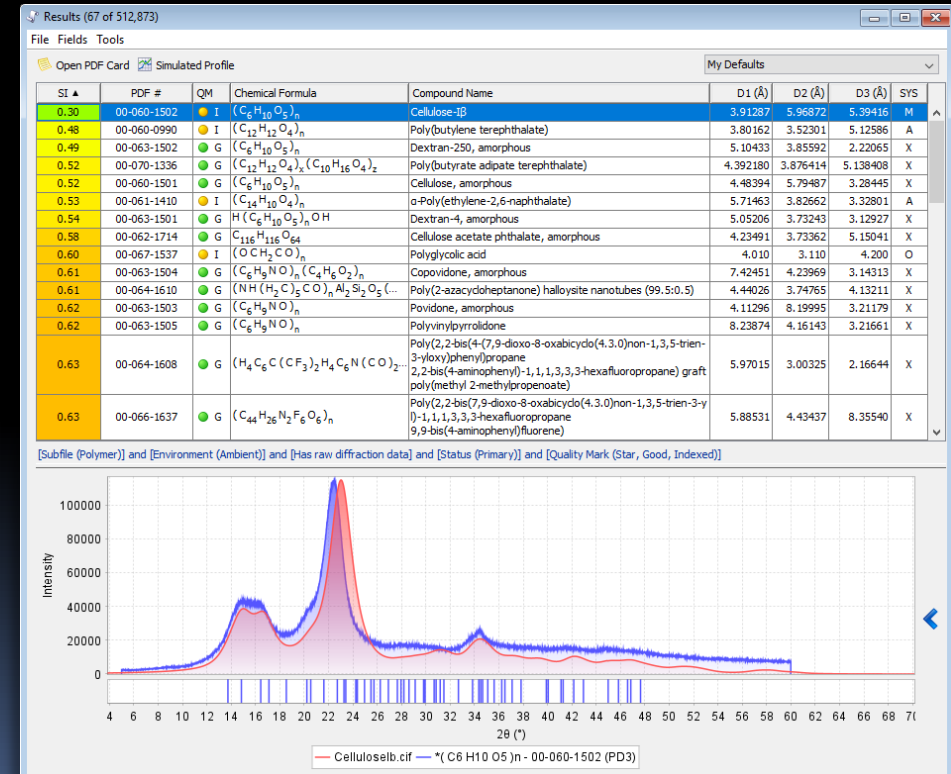
Hits: 1,128

Color Coded Features

Color Coded Bar Charts

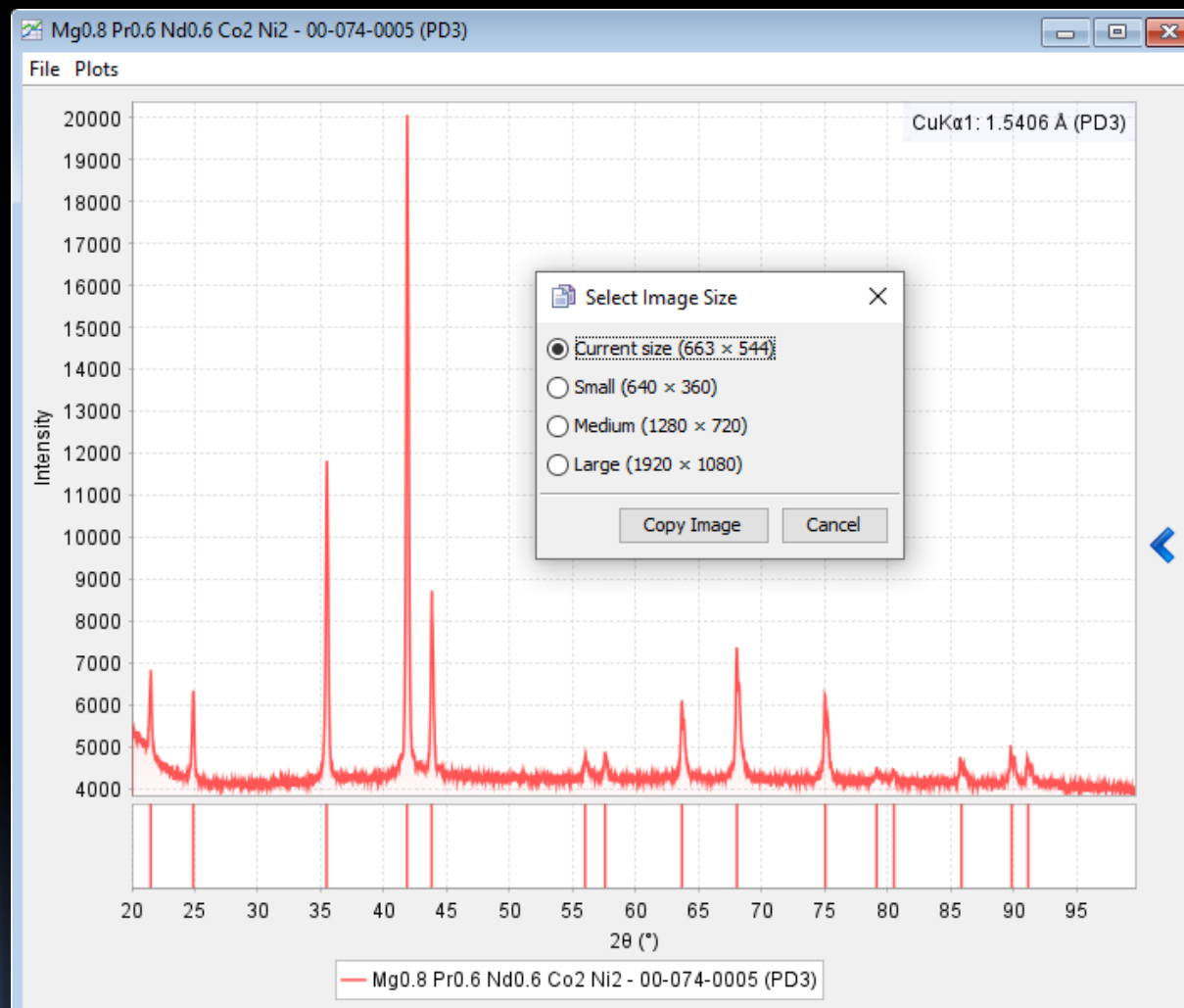


Color Coded GOMs



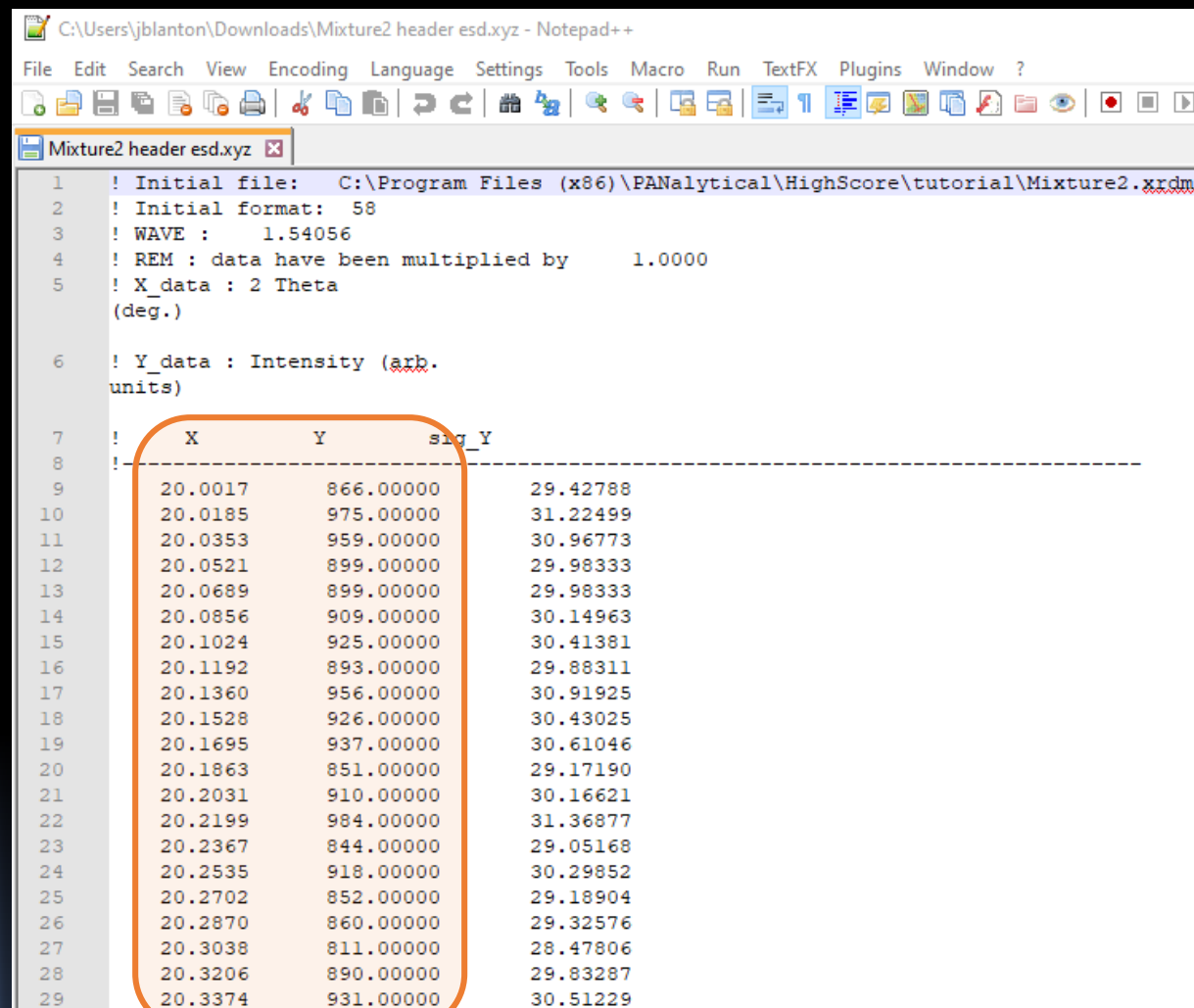
New Graphing Features

- Unzoom button on right side of all x-y graphs
- Quickly save any graph using the right-click menu
 - Includes 2D > 1D diffraction integration*
- Select image resolution when copying or saving a graph image



New Sleeve/Sleeve+ Features

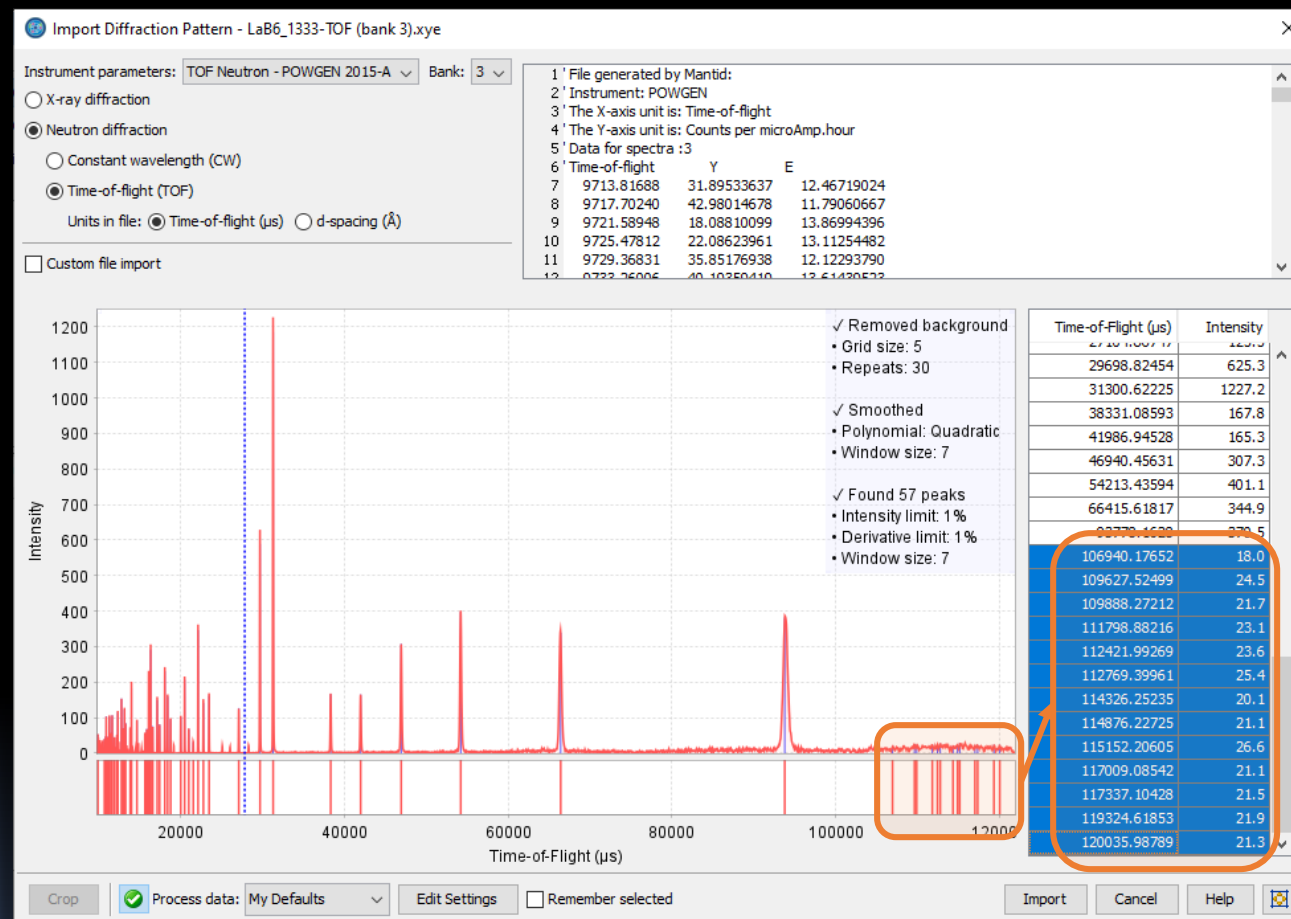
- Added support for new 1D diffraction pattern formats
 - Anton Paar (*.h5)
 - STOE (*.raw)
 - CIF's exported from Jana
- Added support for new 2D diffraction pattern formats*
 - Diamond Light Source (*.h5)
 - MarCCD (*.mccd)
- Automatically detects 2θ and intensity data if file format is not recognized



```
C:\Users\jblanton\Downloads\Mixture2 header esd.xyz - Notepad++
File Edit Search View Encoding Language Settings Tools Macro Run TextFX Plugins Window ?
Mixture2 header esd.xyz x
1 ! Initial file: C:\Program Files (x86)\PANalytical\HighScore\tutorial\Mixture2.xrdsn
2 ! Initial format: 58
3 ! WAVE : 1.54056
4 ! REM : data have been multiplied by 1.0000
5 ! X_data : 2 Theta
  (deg.)
6 ! Y_data : Intensity (arb.
  units)
7 ! X Y sig_Y
8 !-----
9 20.0017 866.00000 29.42788
10 20.0185 975.00000 31.22499
11 20.0353 959.00000 30.96773
12 20.0521 899.00000 29.98333
13 20.0689 899.00000 29.98333
14 20.0856 909.00000 30.14963
15 20.1024 925.00000 30.41381
16 20.1192 893.00000 29.88311
17 20.1360 956.00000 30.91925
18 20.1528 926.00000 30.43025
19 20.1695 937.00000 30.61046
20 20.1863 851.00000 29.17190
21 20.2031 910.00000 30.16621
22 20.2199 984.00000 31.36877
23 20.2367 844.00000 29.05168
24 20.2535 918.00000 30.29852
25 20.2702 852.00000 29.18904
26 20.2870 860.00000 29.32576
27 20.3038 811.00000 28.47806
28 20.3206 890.00000 29.83287
29 20.3374 931.00000 30.51229
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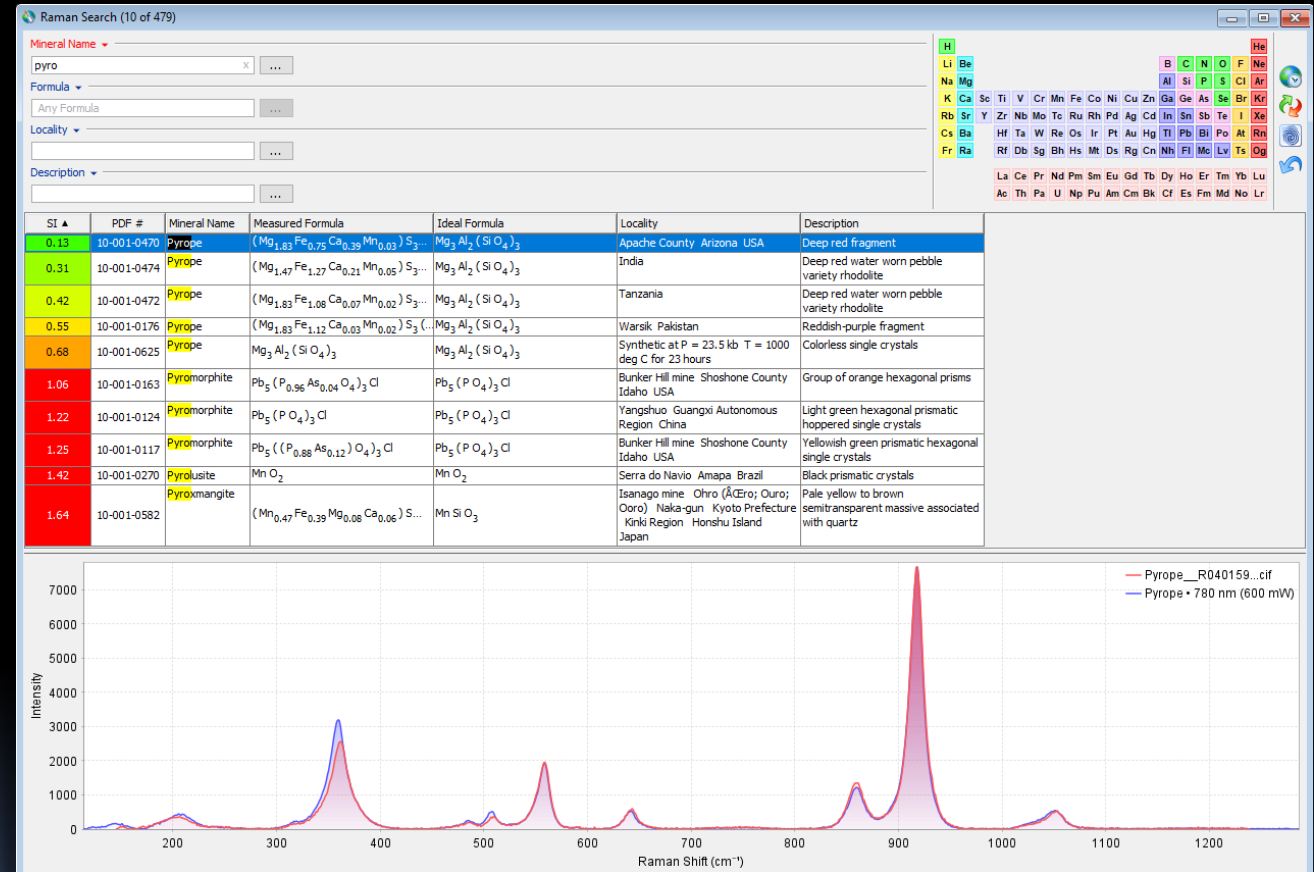
New Sleeve/Sleeve+ Features (cont.)

- Bulk peak edit: Remove peaks directly from the peaks table using a right-click menu
- Add or remove peaks without having to reset the session
- Zoom to peak option for trace phase analysis
- Add phases to a Custom PDF Set
- Sleeve+ project files now save and restore all simulation settings*
 - Geometry settings
 - Profile settings
 - Preferred orientation settings
 - Internal standard settings
 - Isotopic substitutions (neutrons)



Raman Search*

- Dynamic searches for new Raman data
 - Periodic table search
 - Mineral name search
 - Formula search
 - Locality search
 - Description search
- Search values highlighted in table
- Save and retrieve searches
- Import Raman spectra for single-phase ID
 - Supports data processing
- Collaboration with the RRUFF Project (<https://rruff.info>)



Raman PDF Cards*

- Displays Raman data
 - Mineral name
 - Measured formula
 - Ideal formula
 - Locality
 - Description
 - Set 10-xxx-xxxx
- Displays Raman spectra
 - Supports multiple wavelengths (user-selectable)
- Displays cross-references
 - Raman patterns linked to XRD patterns
 - RRUFF ID

