



New Features for Release 2020

New Features for Data Mining

New Features for Data Mining

- New searches and display fields
 - Zeolite name
 - Molecular weight (g/mol)
 - Can be combined with X-ray/neutron/electron diffraction phase ID (Sieve+) and XRF phase ID (Microanalysis)
- Searches can be cancelled at any time

The screenshot displays the 'Search' window with various filters applied. The 'Subfile' dropdown is set to 'test'. The 'Environment' section includes checkboxes for 'Ambient', 'Non-ambient', 'Temp.', 'Press.', and 'Temp. & Press.'. The 'Status' section has checkboxes for 'Primary', 'Alternate', and 'Deleted'. The 'Quality Mark' section includes a 'Star' icon and a list of quality marks: 'Good', 'Indexed', 'Calculate', 'Prototype', 'Minimal', and 'Deleted'. The 'Database' section includes checkboxes for 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'. The 'Periodic Table' and 'Formula' sections are also visible. The search results are displayed in a table with columns: PDF #, QM, Chemical Formula, Compound Name, Zeolite Name, and SYS.

PDF #	QM	Chemical Formula	Compound Name	Zeolite Name	SYS
00-062-0311	● S	C _{0.97} H _{1.21} Al _{0.375} N _{0.24} Na _{0.33} ...	p-N,N-Dimethylnitroaniline	Mordenite	O
00-062-0312	● S	C _{0.97} H _{1.21} Al _{0.375} N _{0.24} Na _{0.33} ...	p-N,N-Dimethylnitroaniline	Mordenite	O
01-072-8429	● B	Na _{7.3} K _{0.2} Al _{8.3} Si _{39.9} O ₉₆	Sodium Potassium Aluminum Silicon Oxide	Mordenite	O
01-083-1338	● B	Ca _{0.32} Ba _{3.32} (Al _{8.6} Si _{39.9} O ₉₆)	Barium Calcium Aluminum Silicon Oxide	Mordenite	O
04-012-8235	● B	K _{1.5} NaCaAl _{4.5} Si _{19.5} O ₄₈ (H ₂ O...	Potassium Sodium Calcium Aluminum Silicon Oxide Hydrate	Mordenite	O

The search criteria are: [Zeolite Name Exactly 'Mordenite'] And [Status (Primary, Alternate)]

New Features for Data Mining

The screenshot shows a software interface for data mining, likely a crystallographic database search tool. The interface includes a search bar, a list of filters (Subfile, Environment, Status, Quality Mark, Database), a periodic table, and a table of results.

Search Window:

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial.
- Environment:** Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, Raw Diffraction Data.
- Status:** Primary, Alternate, Deleted.
- Quality Mark:** Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision.
- Database:** ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05).

Periodic Table: The periodic table is displayed with elements color-coded by group. The search results are shown in a table below the periodic table.

Search Results Table:

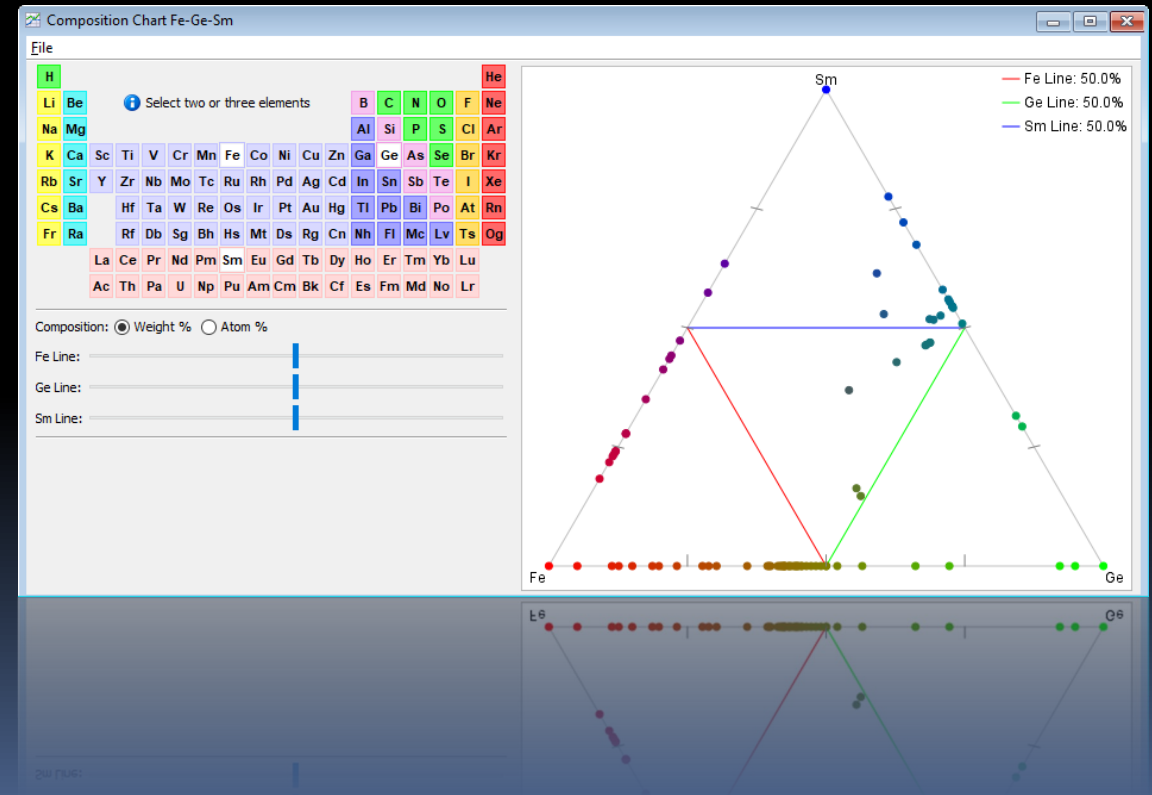
Formula/Name	Hits
Ag	65
Bi _{1.327}	2
Bi	44
Cu	66
Cu _{0.99}	2
Pb	39
S ₈	10
S ₆	1
S	60
Ag _{99.5} Bi _{0.5}	1
Ag _{3.96} Bi _{0.04}	1
Ag _{0.99} Bi _{0.01}	1
Ag _{0.98} Bi _{0.02}	1
Ag _{0.976} Bi _{0.024}	1
Ag _{3.892} Bi _{0.108}	1
Ag _{0.97} Bi _{0.03}	1

Quinary sorting of composition diagram lists

- A, B, C, D, and E compounds (pure elements)
- A-B compounds (sorted by A content)
- A-C compounds (sorted by A content)
- A-D compounds (sorted by A content)
- A-E compounds (sorted by A content)
- B-C compounds (sorted by B content)
- B-D compounds (sorted by B content)
- B-E compounds (sorted by B content)
- C-D compounds (sorted by C content)
- C-E compounds (sorted by C content)
- D-E compounds (sorted by D content)
- A-B-C compounds (sorted by A content)
- A-B-D compounds (sorted by A content)
- A-B-E compounds (sorted by A content)
- A-C-D compounds (sorted by A content)
- A-C-E compounds (sorted by A content)
- B-C-D compounds (sorted by B content)
- B-C-E compounds (sorted by B content)
- C-D-E compounds (sorted by C content)
- A-B-C-D compounds (sorted by A content)
- A-B-C-E compounds (sorted by A content)
- A-B-D-E compounds (sorted by A content)
- A-C-D-E compounds (sorted by A content)
- B-C-D-E compounds (sorted by B content)
- A-B-C-D-E compounds (sorted by A content)

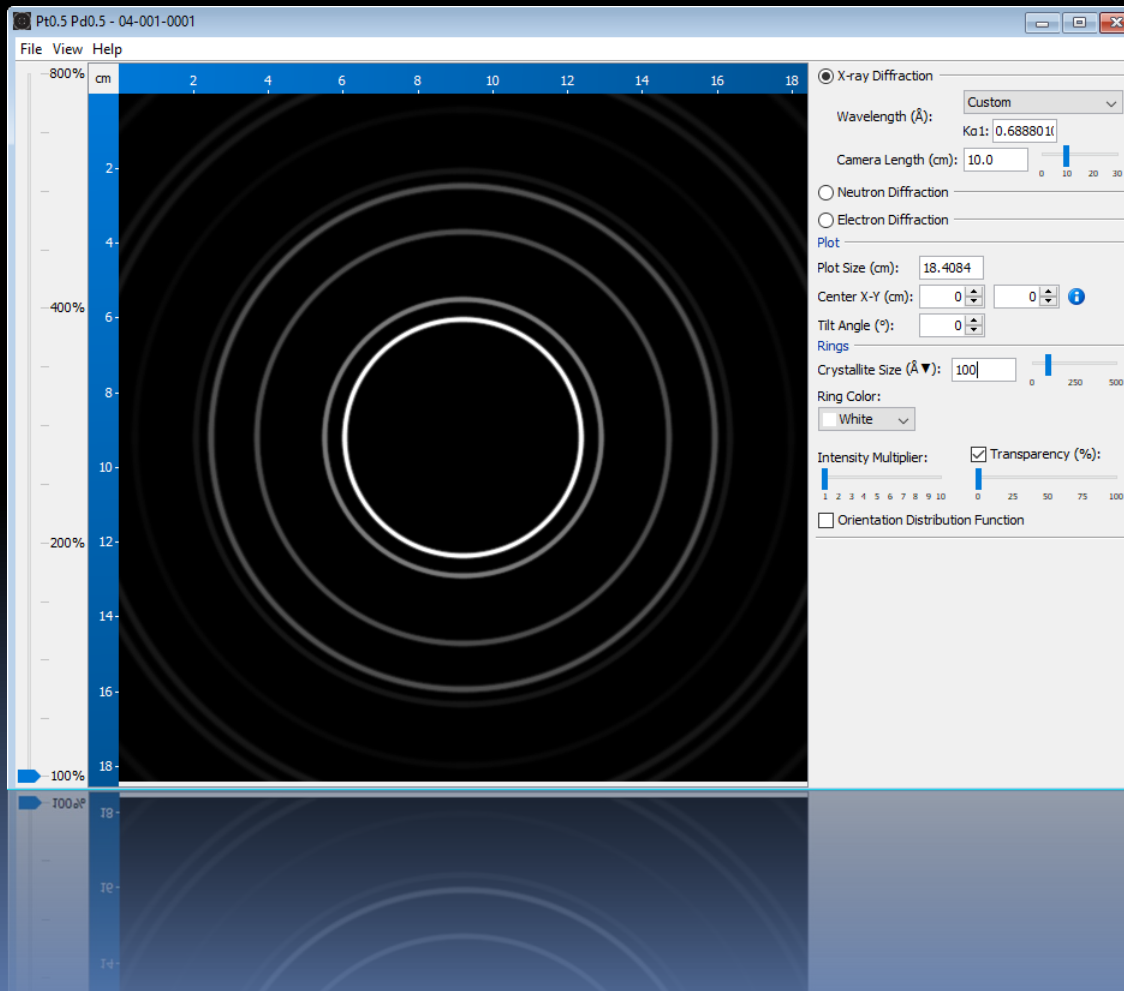
New Features for Data Mining

- Composition graphs
 - Supports binary and ternary systems
 - Color-coded data points
 - Weight % or atomic %
 - User-defined divider lines
 - Tooltips show composition
 - Click to view PDF entries



New Features for Simulations

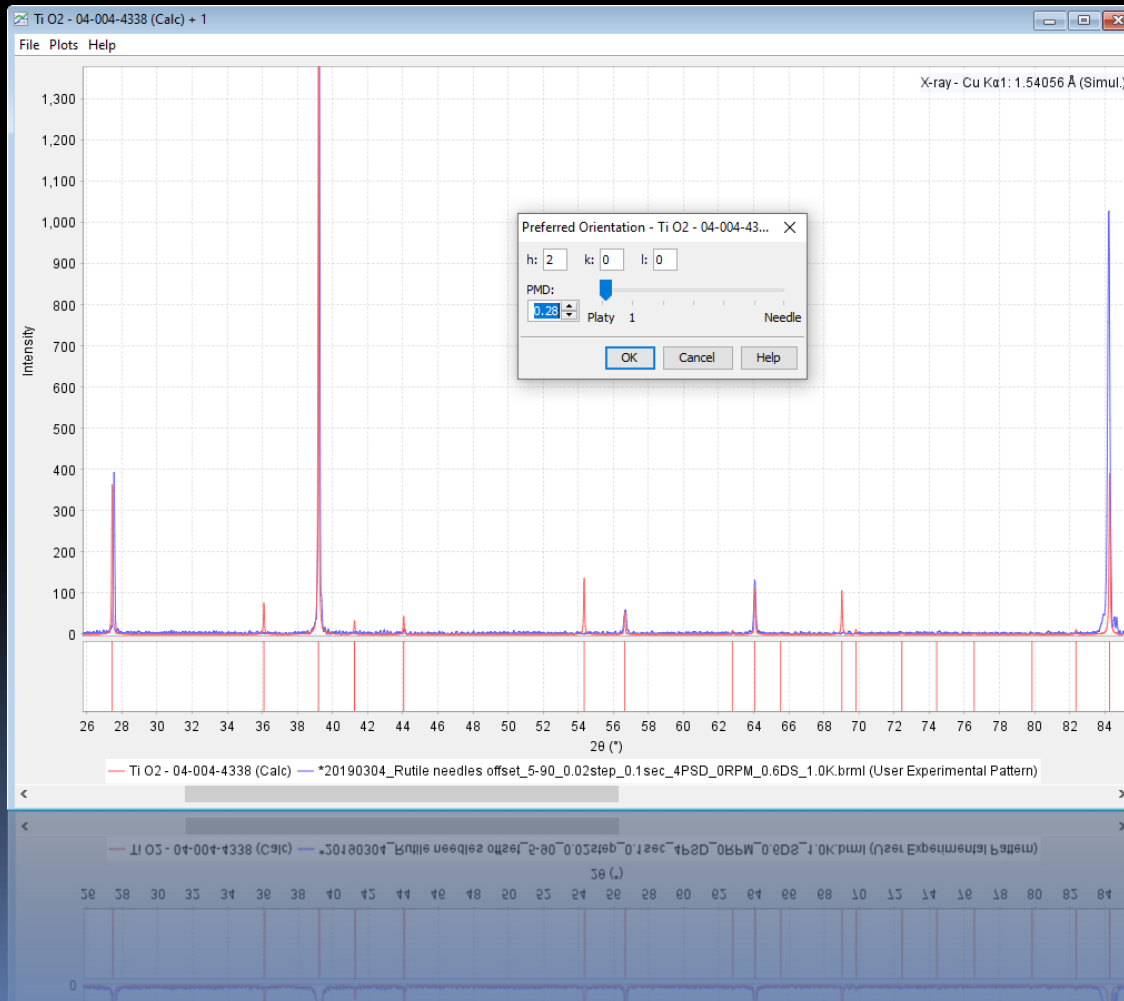
New Features for Simulations



- Export SAED, EBSD, and ring pattern simulations as image files (electron diffraction subcommittee user group suggestion)

- *.jpg
- *.gif
- *.png
- *.tif

New Features for Simulations

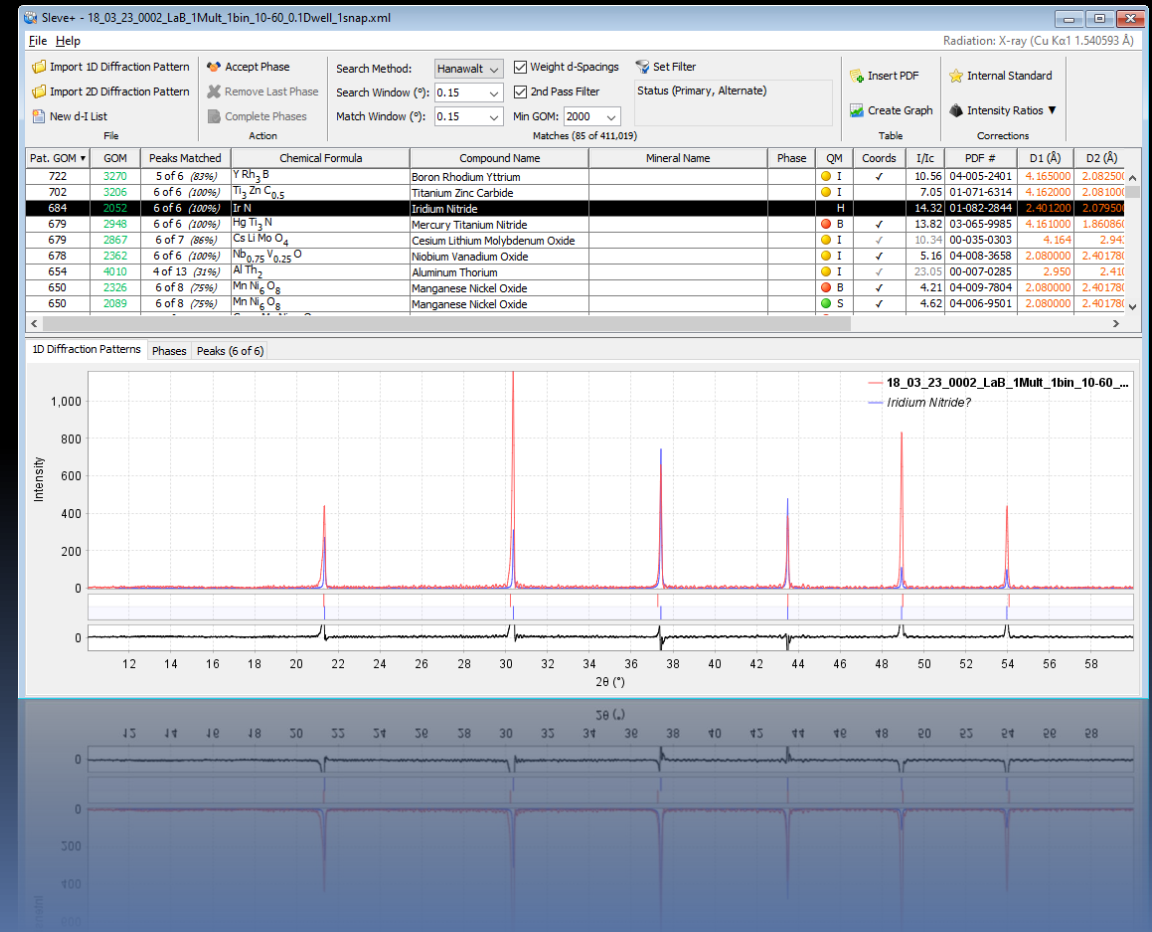


- Dynamic preferred orientation
- Visually compare experimental data with simulated diffraction patterns to determine the amount of preferred orientation.

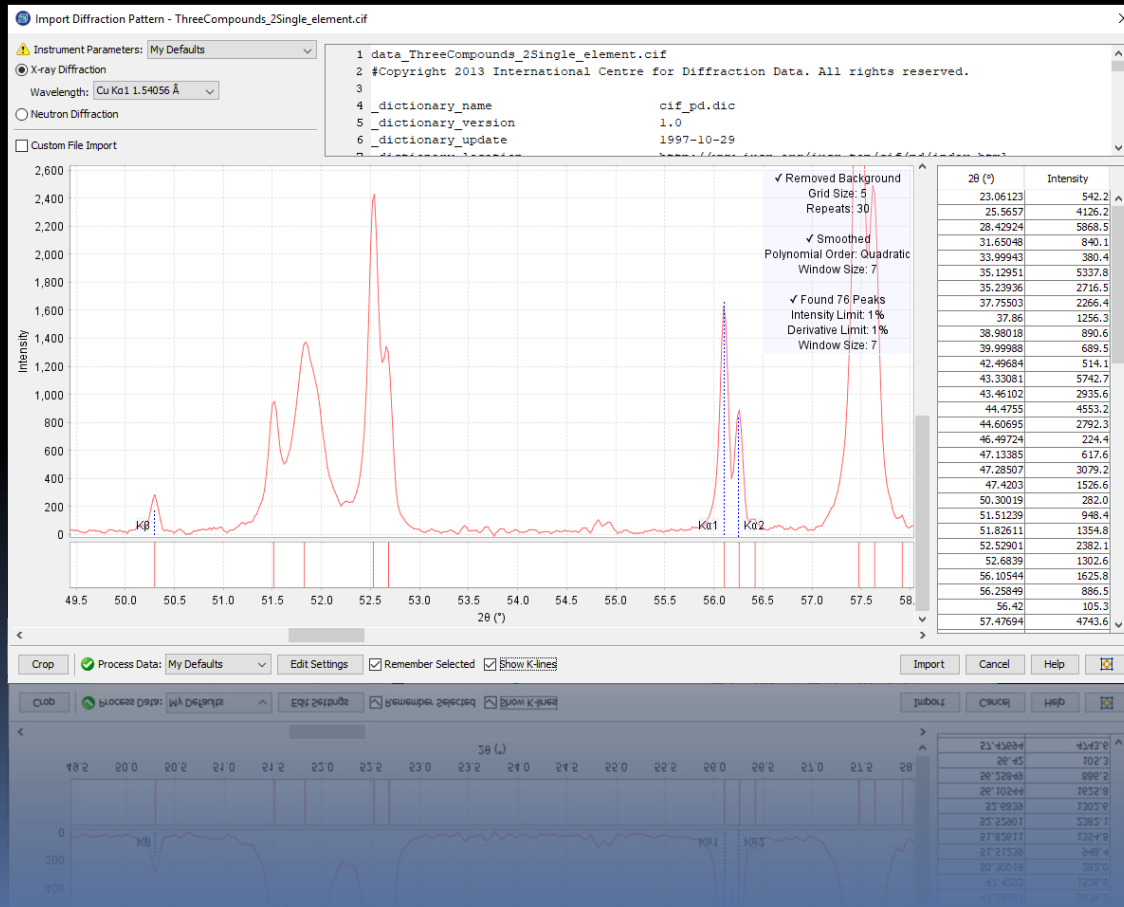
New Features for Phase ID

New Features for Phase ID

- New supported 1D diffraction pattern file types:
 - Proto *.xml files
 - Shimadzu *.raw files
 - MDI *.dif files (processed *.mdi)



New Features for Phase ID



- K-line cursor when processing experimental data
- Shows where a potential $K\alpha_2$ line and $K\beta$ line may exist in relation to the user-defined $K\alpha_1$ line using the mouse cursor position

New Features for Phase ID

- Importing 2D diffraction patterns
 - User-defined color palette for better contrast
 - 2D-to-1D integration now supports multi-core processors

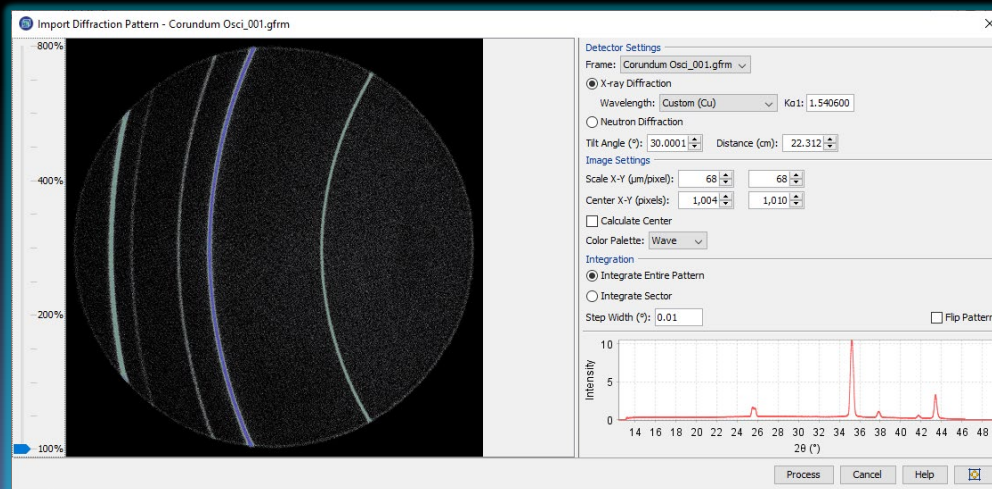
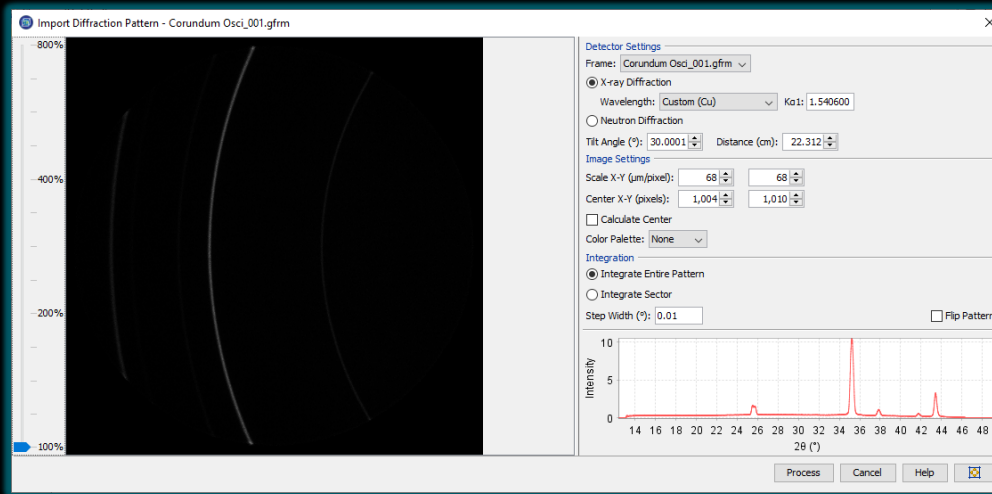
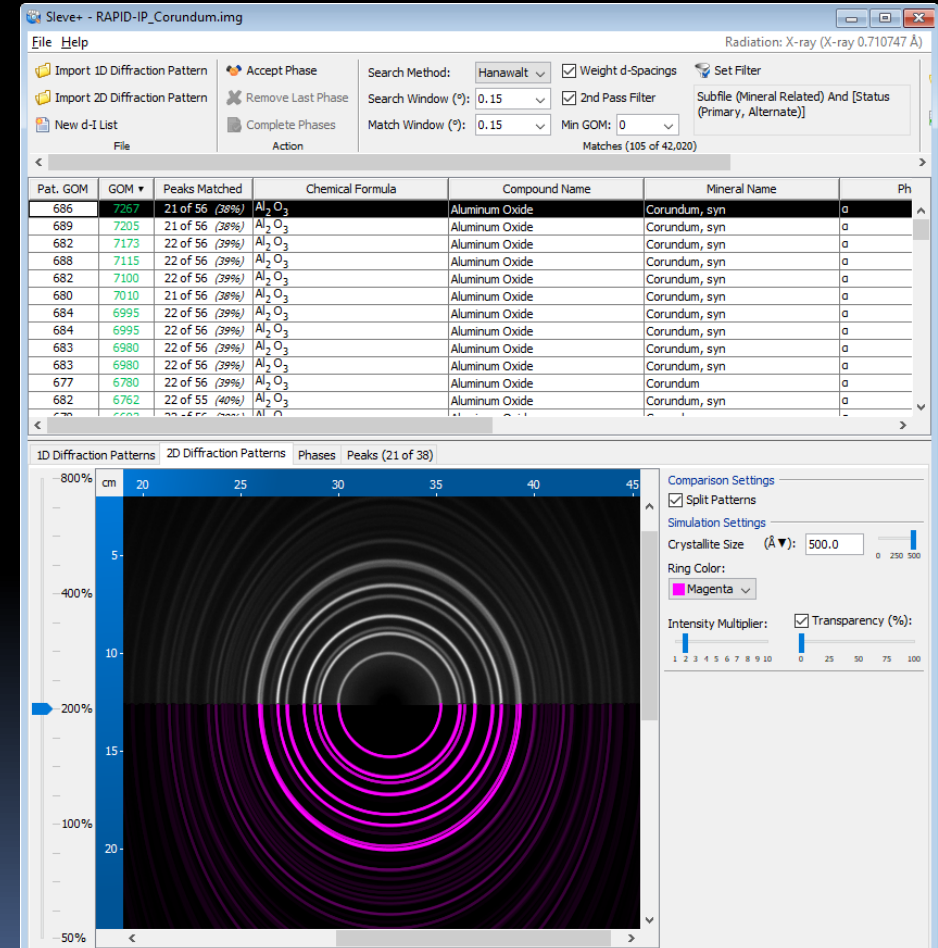


	Image Size	2019	2020
Bruker	2048 x 2048	10s	4s
DECTRIS Eiger	3110 x 3269	26s	10s
Rigaku	4600 x 2560	24s	12s

New Features for Phase ID

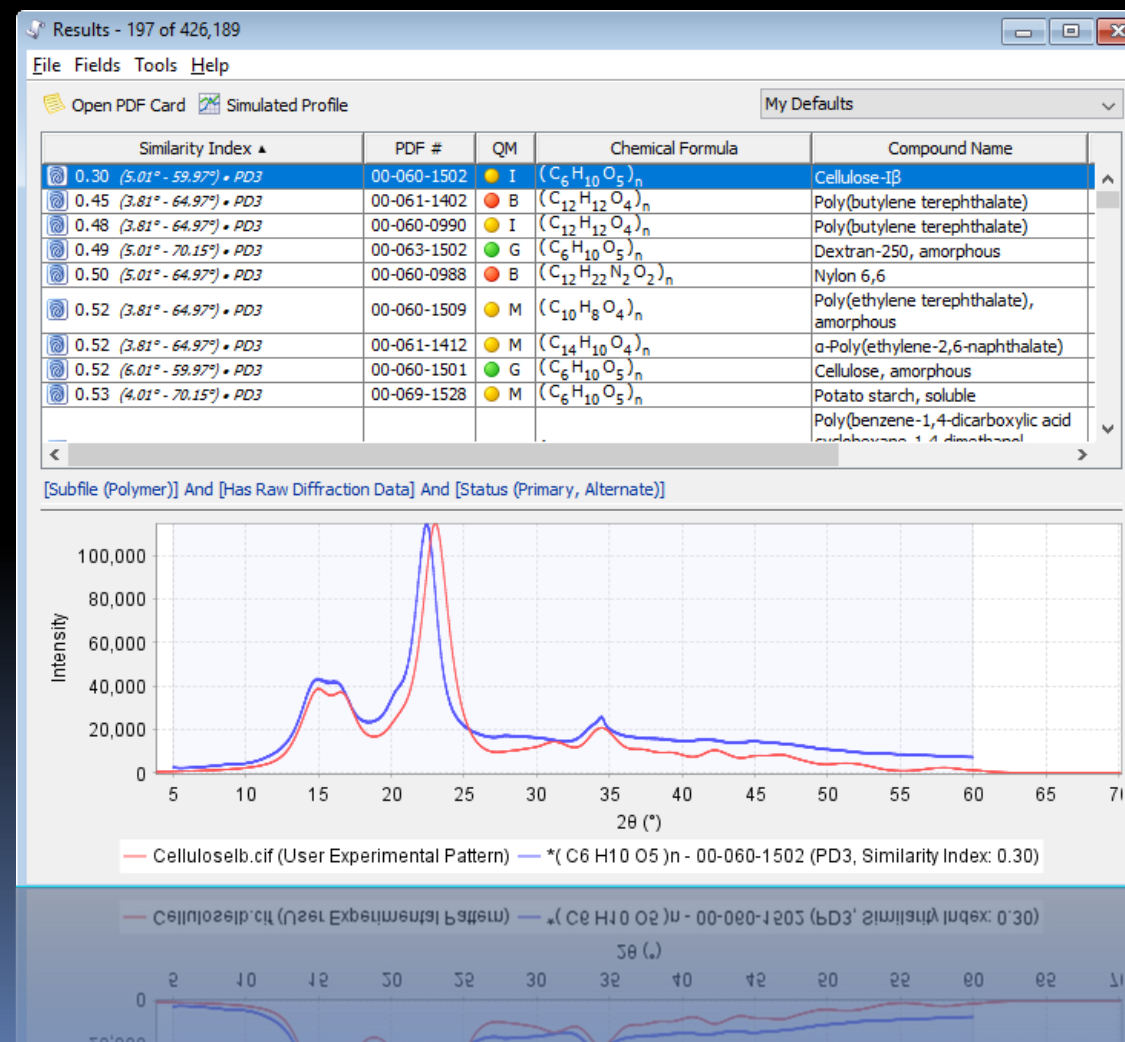
- Compare 2D diffraction pattern images directly in Sleeve+
- Split view for easier comparison
- Dynamically change crystallite size of 2D simulations
- Increase intensity brightness for 2D simulations
- Support comparison of multiple 2D frames



New Features for Phase ID

- Similarity indexes now support multi-core processors

	# Entries	2019	2020
Depressants	213	10s	3s
Clays	335	33s	20s
Polymers	1,336	25s	13s



New System-Wide Features

- More accurate d-spacing precision
- Custom program font size
 - 100%
 - 125%
 - 150%
 - 175%

Results - 16,260 of 412,083

File Fields Tools Help

Open PDF Card Simulated Profile My Defaults

PDF #	QM	Chemical Formula	Compound Name	D1 (Å)	D2 (Å)	D3 (Å)	SYS
00-001-0363	• I	(NH ₄) ₂ SO ₄	Ammonium Sulfate	4.36	3.12	3.03	O
00-001-0538	• I	Sb ₂ S ₃	Antimony Sulfide	3.57	1.92	3.02	O
00-001-0937	• I	Sr Zr O ₃	Strontium Zirconium Oxide	2.90	1.67	2.04	C
00-001-1029	• I	Ca ₂ SiO ₄	Calcium Silicate	2.74	3.01	1.90	O
00-002-0374	• I	Sb ₂ S ₃	Antimony Sulfide	3.55	1.94	1.69	O
00-002-1280	• B	Ni S	Nickel Sulfide	1.97	2.96	1.71	H
00-002-1450	• I	In N	Indium Nitride	1.069	2.700	1.134	H
00-003-0368	• I	Ca S O ₄	Calcium Sulfate	3.49	2.78	1.84	O
00-003-0567	• I	K Ca F ₃	Potassium Calcium Fluoride	3.09	2.19	1.78	C
00-003-0864	• B	Co Fe ₂ O ₄	Cobalt Iron Oxide	2.53	1.48	1.61	C
00-003-0965	• B	Al Fe ₃ C _{0.69}	Aluminum Iron Carbide	2.160	1.890	1.330	C
00-003-1102	• B	Ba Th O ₃	Barium Thorium Oxide	1.8400	0.8820	3.1800	C
00-004-0545	• S	Ge	Germanium	2.2660	2.0000	1.7060	C

[Subfile (Ceramic)] And [Status (Primary, Alternate)]

[Subfile (Ceramic)] And [Status (Primary, Alternate)]

00-003-1105	• B	Ba Th O ₃	Barium Thorium Oxide	1.8400	0.8820	3.1800	C
00-003-0965	• B	Al Fe ₃ C _{0.69}	Aluminum Iron Carbide	2.160	1.890	1.330	C
00-003-0864	• B	Co Fe ₂ O ₄	Cobalt Iron Oxide	2.53	1.48	1.61	C