



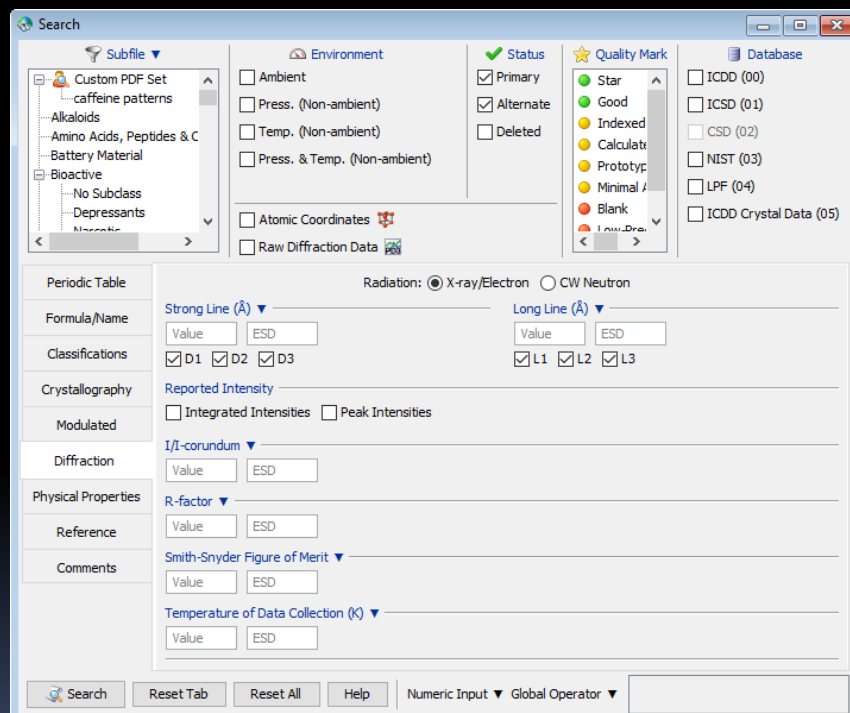
NEW FEATURES FOR RELEASE 2018

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:

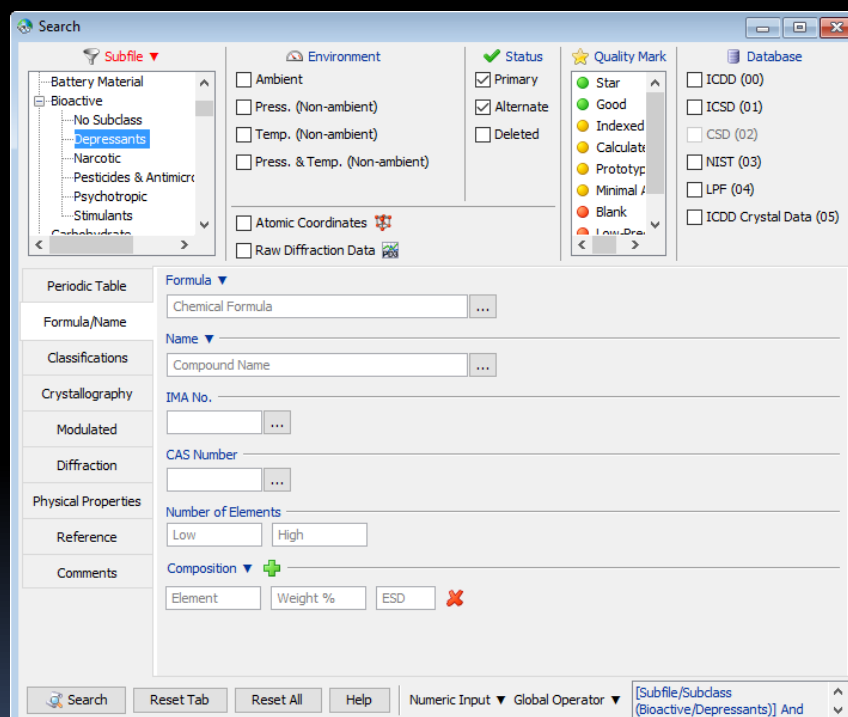
- ✔ Data Mining Enhancements
- ✔ PDF Card Enhancements
- ✔ Graphing Enhancements
- ✔ New Pattern Simulation Features
- ✔ Sleve+ Improvements
- ✔ Neutron Diffraction Enhancements

Data Mining



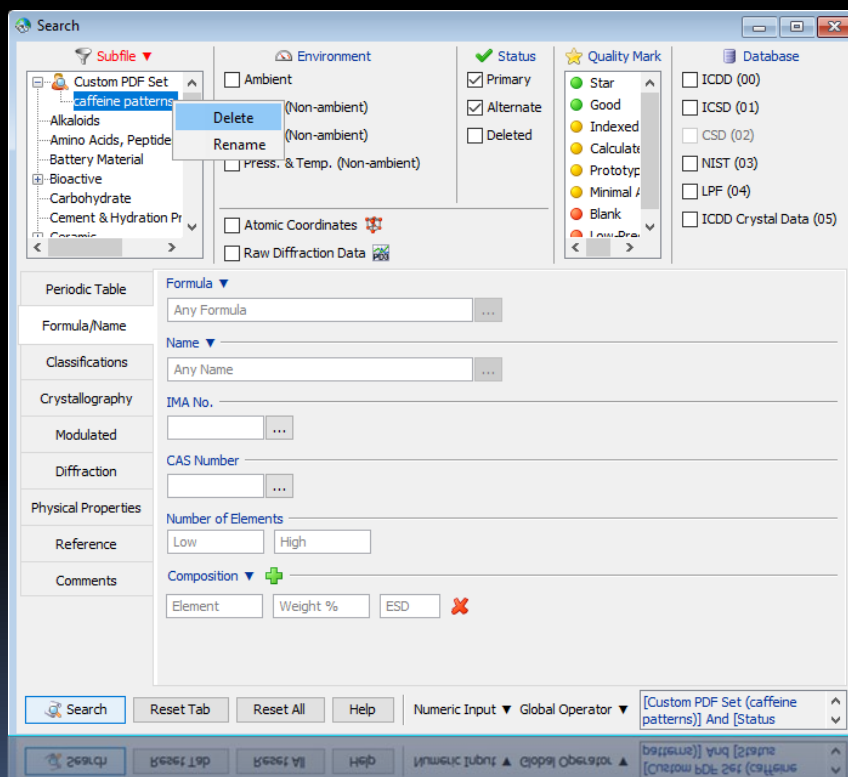
- ✔ Reported Intensity search
 - Peak Intensities
 - Integrated Intensities
- ✔ Subfiles display field*
- ✔ Metals & Alloys – Standard Index*
 - Based on the accepted Linus Pauling File (LPF) prototype structure for each material
 - Empirical Formula [Std.]
 - Space Group
 - Z [Std.]
 - Wyckoff Seq.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

Data Mining



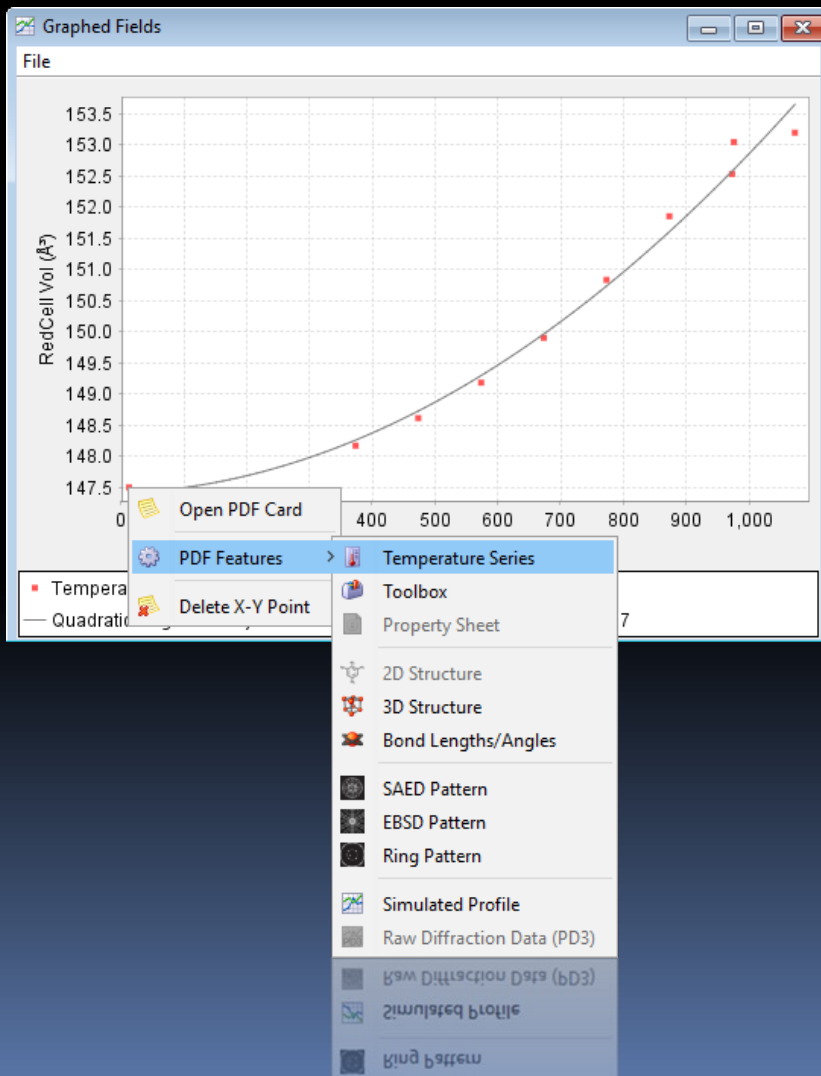
- ✓ New Bioactive subclasses
 - Depressants
 - Pesticides & Antimicrobials
 - Stimulants
- ✓ New Mineral subclass
 - Clays
- ✓ IMA number search

Custom PDF Sets



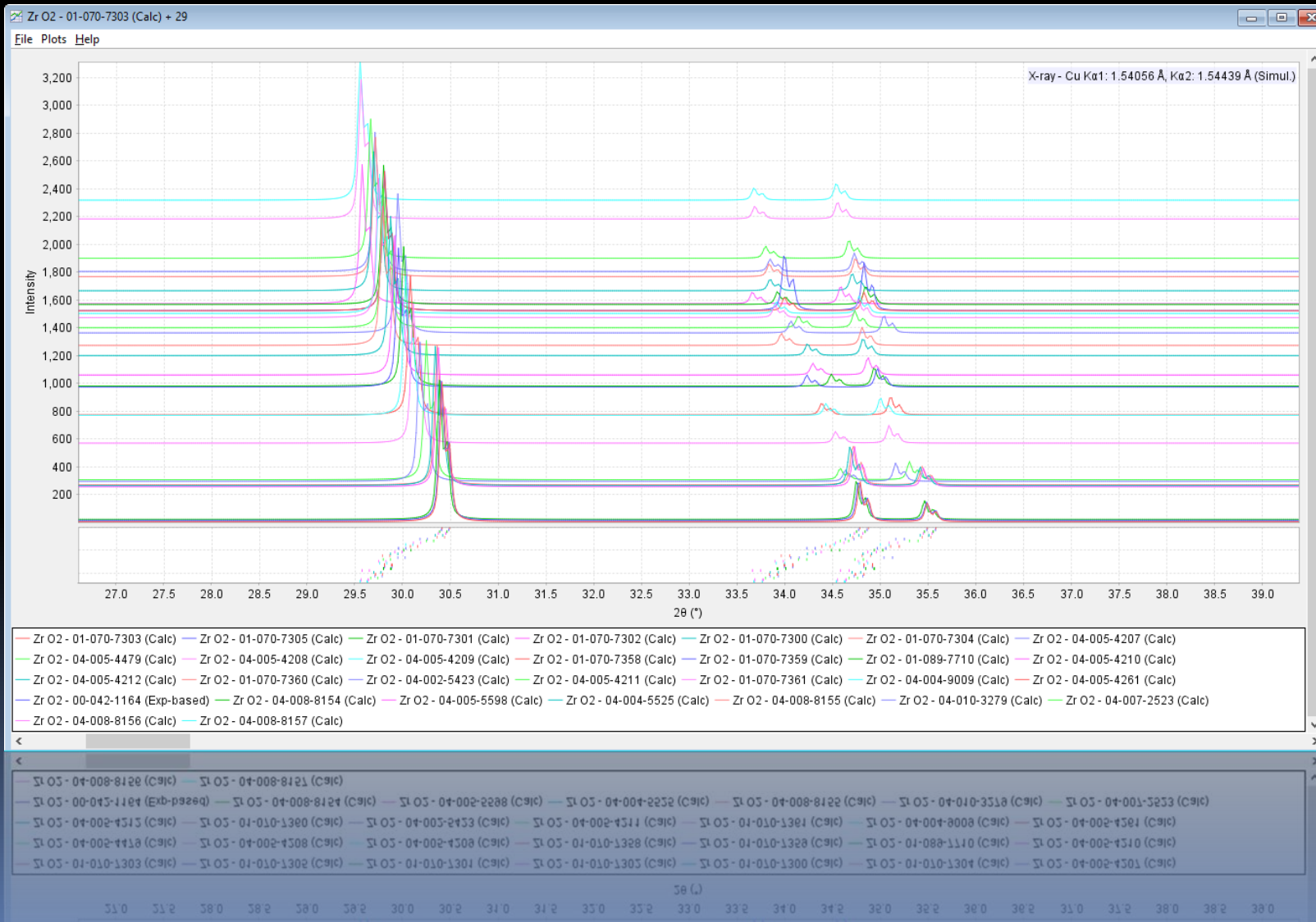
- ✓ User-defined sets of PDF entries
- ✓ Right-click Custom PDF Sets in search form to delete or rename

Data Mining Graphs

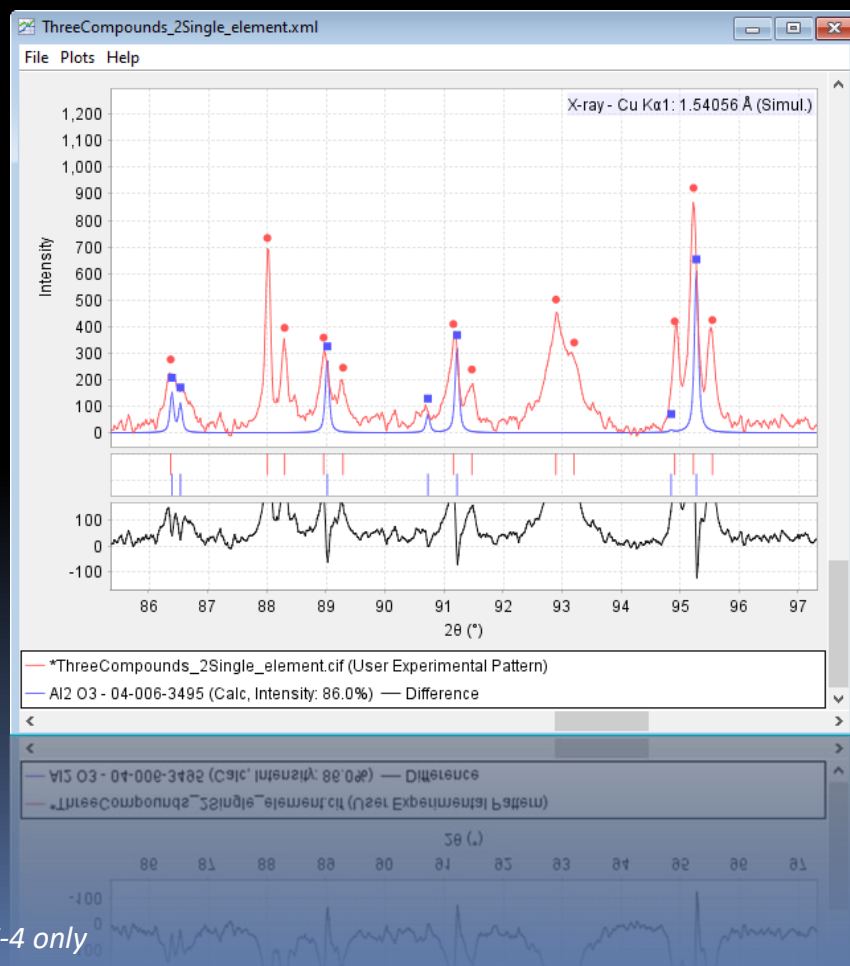


- ✔ Each x-y point represents a PDF entry
- ✔ Right-click x-y points for tool/simulations
 - 3D structures
 - Ring patterns
 - Etc...
- ✔ Manually delete outliers

Temperature Series Intensity Offsets

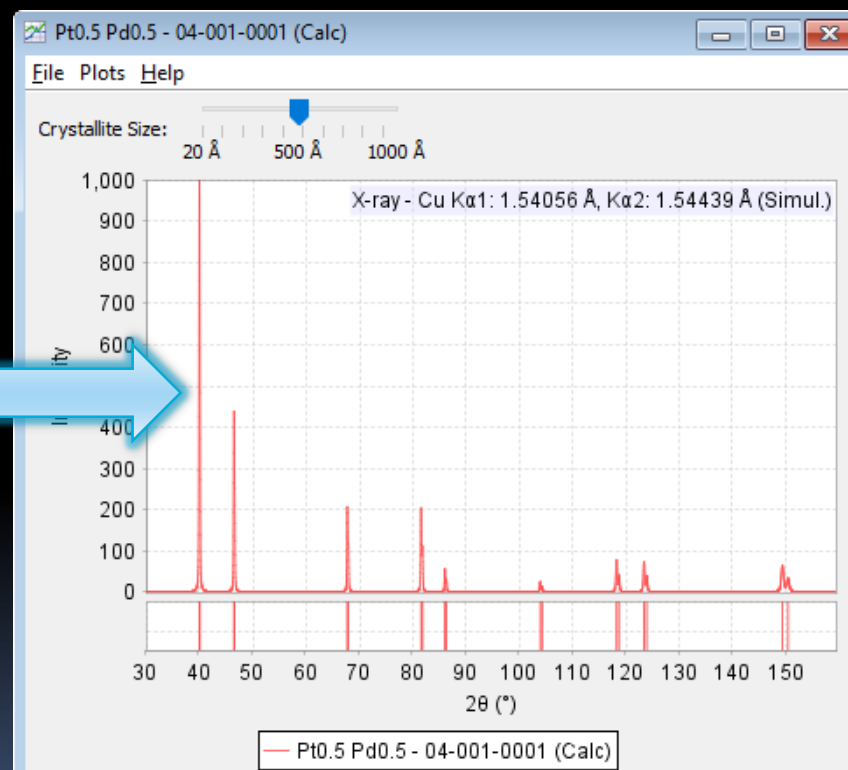
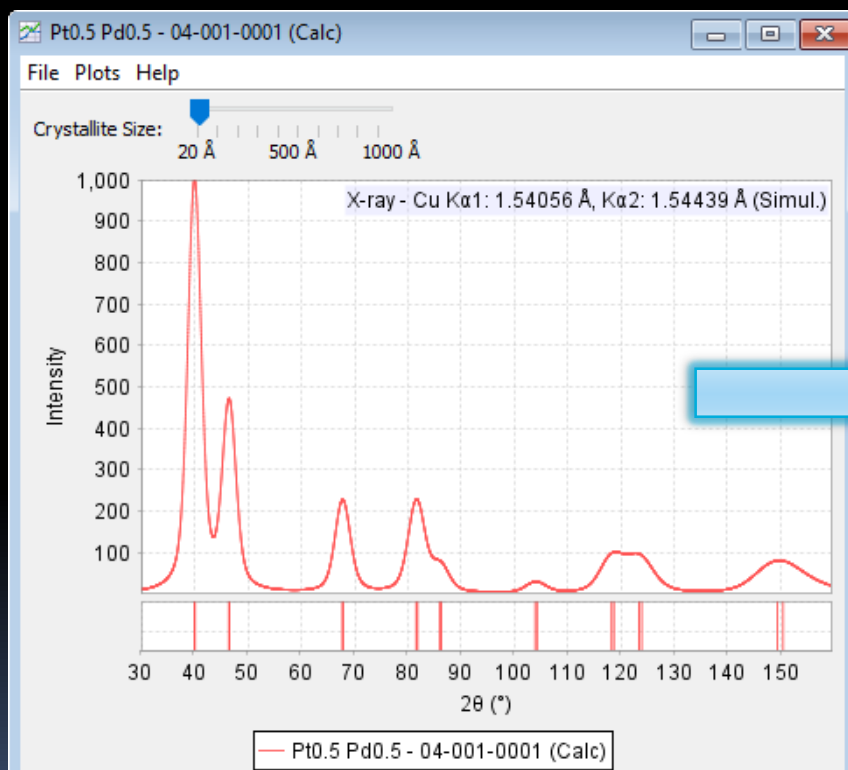


Diffraction Pattern Simulations

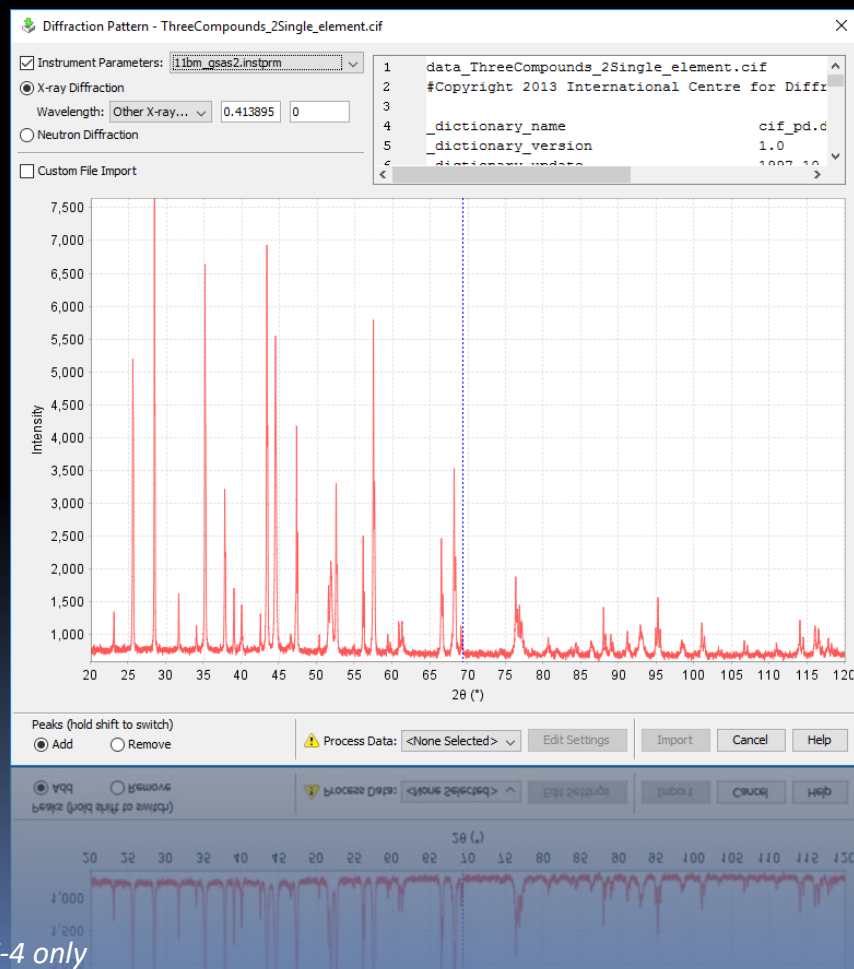


- ✓ Show peak symbols at **top of peaks**
 - Allows phase distinction in B&W publications
- ✓ Line Width and Font settings **saved** between program sessions
- ✓ Tooltips in graph legend display **geometry** and **profile function** settings*

Crystallite Size Slider for Estimation*

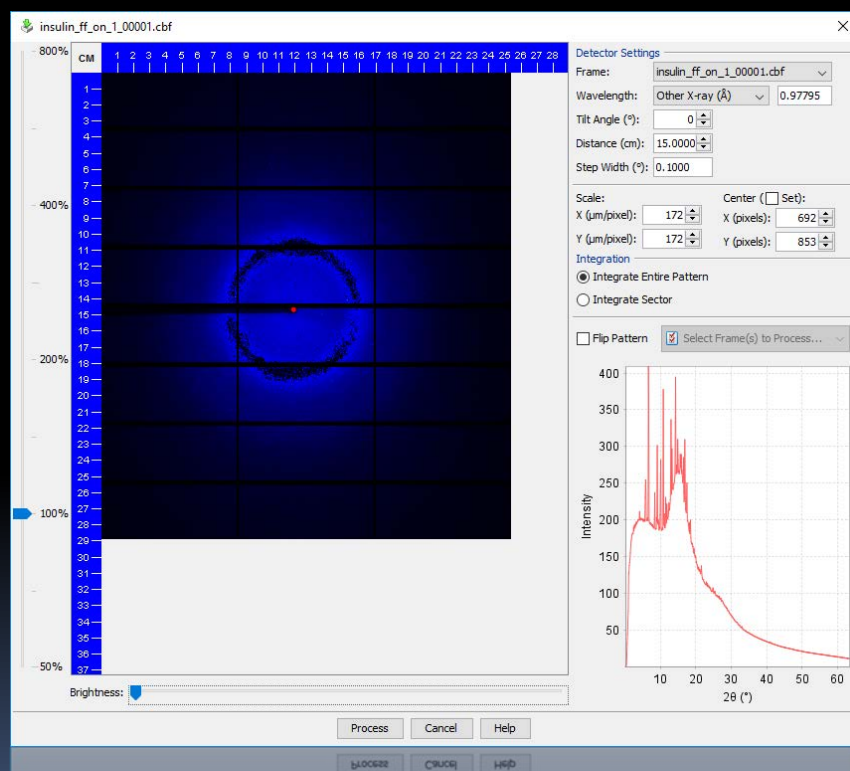


Importing Diffraction Data



- ✓ When importing experimental data, choose instrument parameters from **synchrotron** and **neutron** beamlines (FullProf, GSAS, GSAS-II)*
 - Necessary for accurate diffraction pattern simulations
- ✓ User-defined **$K\alpha_1/K\alpha_2$** for removing the $K\alpha_2$ profile
- ✓ User-defined **2θ zero correction**
- ✓ User-defined **stop line** for importing custom experimental data files
 - **Good for multi-bank data!**

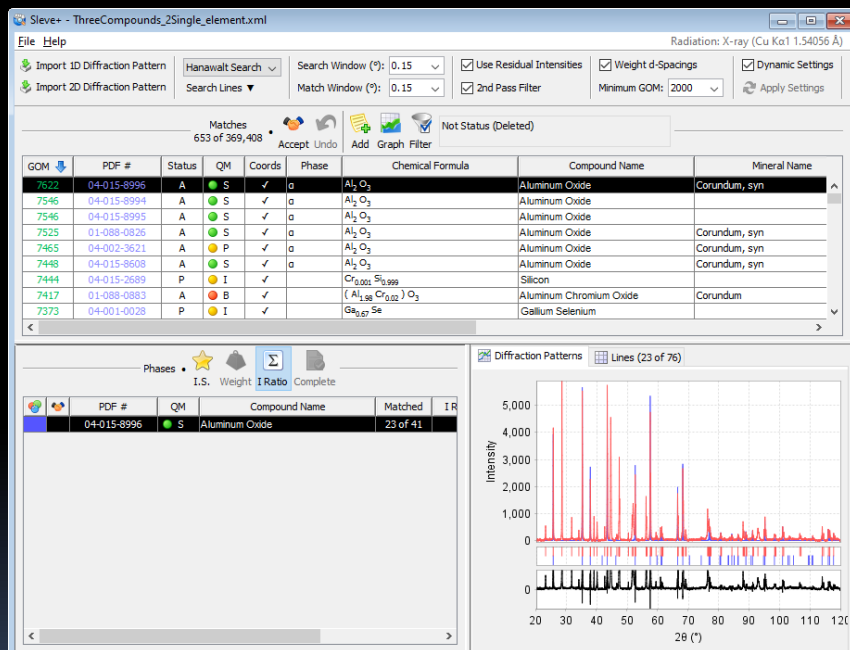
Importing Diffraction Data



- ✔ 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

Sieve/Sieve+ Dynamic Settings



The screenshot shows the Sieve+ software interface with the following settings and data:

Search Settings:

- Search Window (?): 0.15
- Match Window (?): 0.15
- Use Residual Intensities:
- Weight d-Spacings:
- Dynamic Settings:
- 2nd Pass Filter:
- Minimum GOM: 2000

Search Results Table:

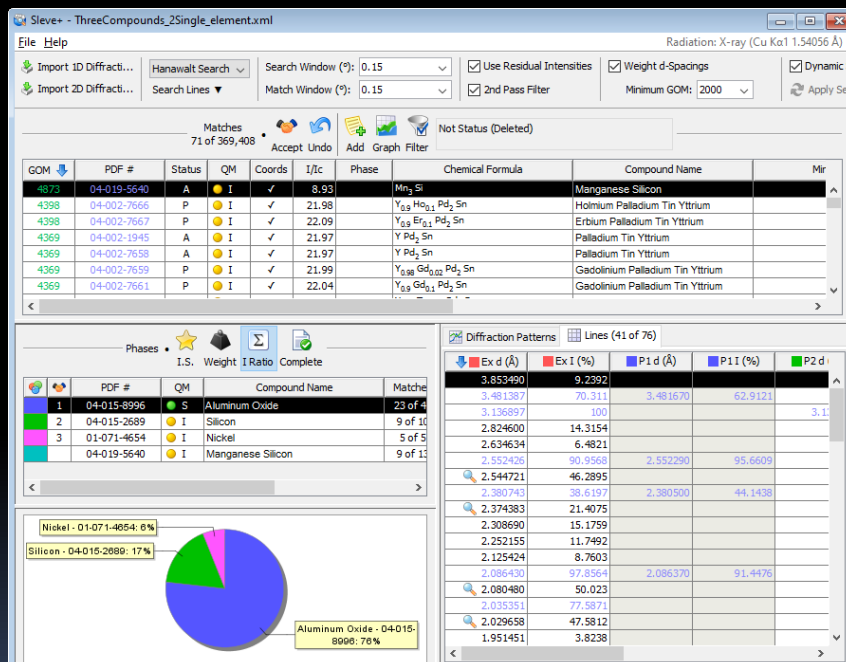
GOM	PDF #	Status	QM	Coords	Phase	Chemical Formula	Compound Name	Mineral Name
7622	04-015-8996	A	S	✓	α	Al ₂ O ₃	Aluminum Oxide	Corundum, syn
7546	04-015-8994	A	S	✓	α	Al ₂ O ₃	Aluminum Oxide	
7546	04-015-8995	A	S	✓	α	Al ₂ O ₃	Aluminum Oxide	
7525	01-088-0826	A	S	✓	α	Al ₂ O ₃	Aluminum Oxide	Corundum, syn
7465	04-002-3621	A	P	✓	α	Al ₂ O ₃	Aluminum Oxide	Corundum, syn
7448	04-015-8608	A	S	✓	α	Al ₂ O ₃	Aluminum Oxide	Corundum, syn
7444	04-015-2689	P	I	✓		Cr _{0.003} Si _{0.999}	Silicon	
7417	01-088-0883	A	B	✓		(Al _{1.98} Cr _{0.02}) ₂ O ₃	Aluminum Chromium Oxide	Corundum
7373	04-001-0028	P	I	✓		Ga _{0.67} Se	Gallium Selenium	

Diffraction Patterns:

The bottom right panel shows a diffraction pattern plot with Intensity on the y-axis (0 to 5,000) and 2θ (°) on the x-axis (20 to 120). The plot displays a series of sharp peaks characteristic of a crystalline material, with the most intense peak at approximately 35° 2θ.

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

Sieve/Sieve+ Features



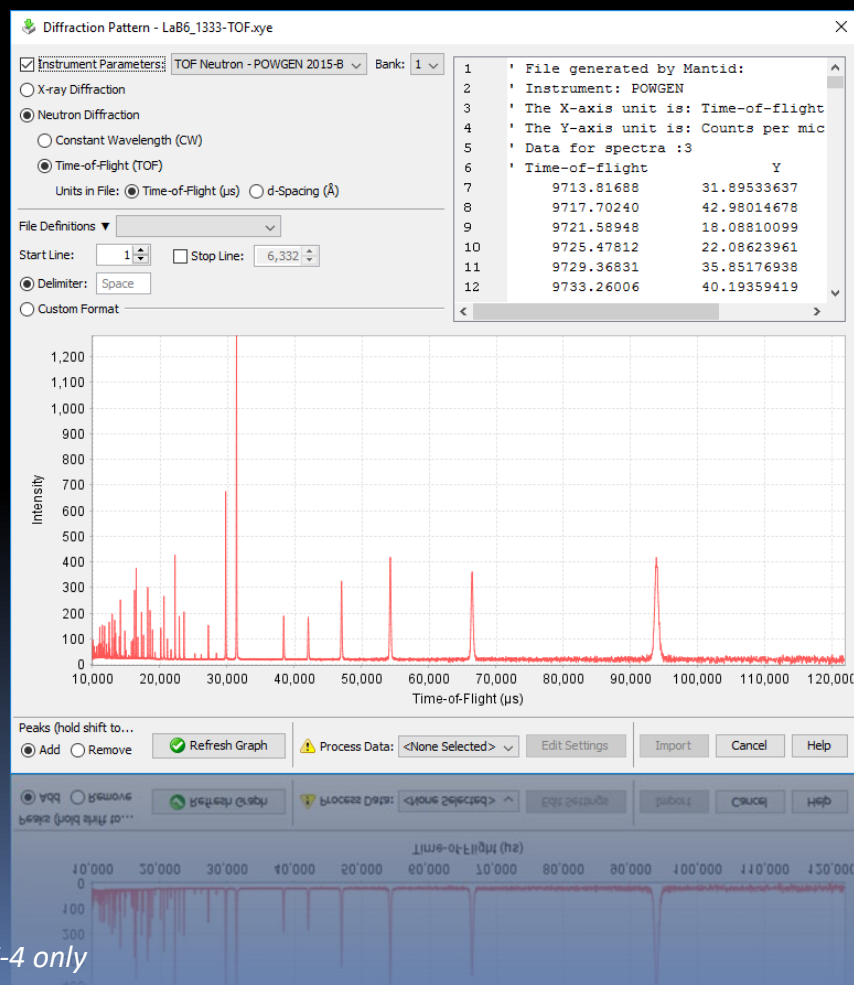
The screenshot displays the Sieve+ software interface with the following components:

- Search Parameters:** Radiation: X-ray (Cu Kα1 1.54056 Å), Search Window (°): 0.15, Match Window (°): 0.15, Use Residual Intensities, Weight d-Spacings, Dynamic S, 2nd Pass Filter, Minimum GOM: 2000.
- Matches Table:** 71 of 369,408 matches. Columns include GOM, PDF #, Status, QM, Coords, I/Ic, Phase, Chemical Formula, Compound Name, and Mir.
- Phases Table:** Lists phases with PDF #, QM, Compound Name, and Matches.

PDF #	QM	Compound Name	Matches
04-015-8996	S	Aluminum Oxide	23 of 4
04-015-2689	I	Silicon	9 of 11
01-071-4654	I	Nickel	5 of 5
04-019-5640	I	Manganese Silicon	9 of 11
- Diffraction Patterns:** Lines (41 of 76). Columns include Ex d (Å), Ex I (%), P1 d (Å), P1 I (%), and P2 d.
- Phase Analysis:** Pie charts showing the relative contribution of phases: Aluminum Oxide - 04-015-8996: 76%, Silicon - 04-015-2689: 17%, Nickel - 01-071-4654: 6%.

- ✓ 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 (LaB₆)
 - NIST SRM 675 (Mica)
 - NIST SRM 676 (Al₂O₃)

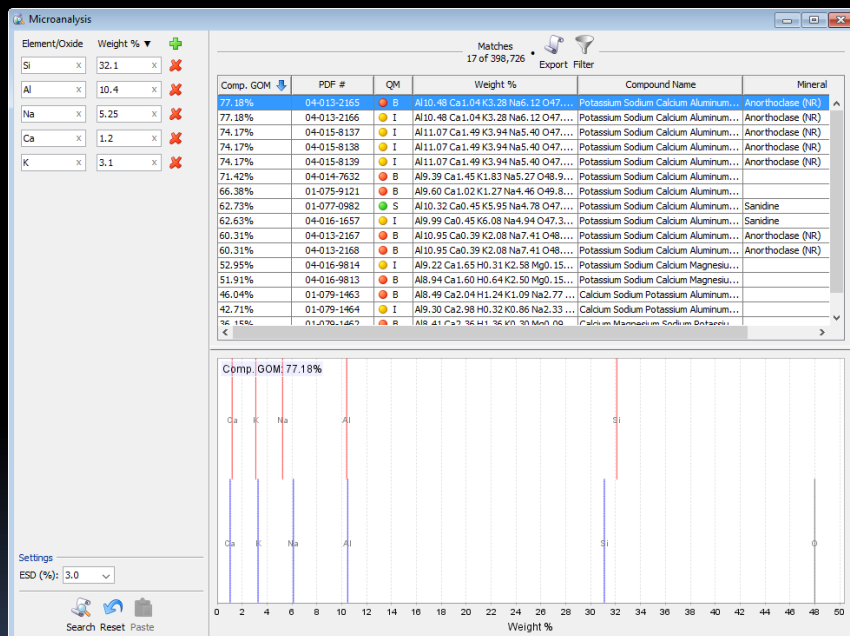
Importing Time-of-Flight (TOF) Neutron Data*



- ✓ 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

Results - 2,247 of 398,726

File Tools Display Fields: My Defaults Help

PDF #	Chemical Formula	Compound Name
00-004-0157	$C_{11}H_{17}NO_3 \cdot 0.5H_2SO_4 \cdot 2H_2O$	Mescaline sulfate dihydrate
00-004-0232	$C_9H_{13}NO_3$	Epinephrine
00-005-0081	$C_{12}H_{16}N_2O_3$	5-Ethyl-5-cyclohexenyl barbituric acid
00-005-0082	$C_{20}H_{24}N_2O_2$	Quinidine
00-005-0087	$C_{11}H_{18}N_2O_3$	Pentobarbital
00-005-0103	$C_{10}H_{16}N_2O_3$	Butethal
00-005-0111	$C_8H_{12}N_2O_3$	Barbital
00-005-0173	$C_{12}H_{12}N_2O_3$	Phenobarbital
00-005-0174	$C_{21}H_{27}NO \cdot HBr$	Isomethadone hydrobromide
00-005-0178	$C_{36}H_{42}N_2O_6 \cdot H_2SO_4 \cdot 5H_2O$	Codeine sulfate pentahydrate
00-005-0179	$C_{34}H_{38}N_2O_6 \cdot H_2SO_4 \cdot 5H_2O$	Morphine sulfate pentahydrate
00-005-0198	$C_{12}H_{12}N_2O_3$	Phenobarbital
00-005-0208	$C_{12}H_{12}N_2O_3$	Phenobarbital
00-005-0324	$C_{12}H_{12}N_2O_3$	Phenobarbital
00-005-0345	$C_{18}H_{21}NO_3 \cdot H_3PO_4 \cdot 2H_2O$	Codeine phosphate dihydrate
00-005-0435	$H_3CO C_{11}H_5O_3$	Methoxsalen
00-006-0015	$C_{18}H_{21}NO_3 \cdot 2H_2O$	Methylidihydromorphinone dihydrate
00-006-0016	$C_{16}H_{23}NO_2$	Propylketobemidone
00-006-0018	$C_{20}H_{23}NO_4 \cdot HCl$	Dihydrocodeinoneenol acetate
00-006-0019	$C_{18}H_{19}NO_3 \cdot HCl$	Morphothebaine hydrochloride
00-006-0023	$C_{24}H_{25}NO_3 \cdot HCl$	Benzylmorphine hydrochloride
00-006-0027	$C_{15}H_{21}NO_2$	Meperidine
00-006-0031	$C_{21}H_{27}NO$	d-l-dl-Methadone
00-006-0035	$C_{17}H_{17}NO_2 \cdot HCl \cdot 0.5H_2O$	Apomorphine hydrochloride hemihydr...
00-006-0038	$C_{15}H_{21}NO_2 \cdot HCl$	Meperidine hydrochloride
00-006-0041	$C_{24}H_{25}NO_3$	Benzylmorphine

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

✔ Formulas use **subscripts** and **superscripts** for proper notation and readability

- ❑ Chemical Formula
- ❑ Empirical Formula
- ❑ Structural Formula

Printing Reports

Mg C O3 · 3 H2 O - 00-001-0130 - Print Preview

Report Export Help

150%

Atomic %: C7.14 · H42.86 · Mg7.14 · O42.86 **Compound Name:** Magnesium Carbonate Hydrate Oxide
Mineral Name: Nesquehonite **Entry Date:** 09/01/1951 **Last Modification Date:** 09/01/2003
Last Modifications: Quality

Radiation: MoKα1 (0.7093 Å) **Filter:** ZrO2 Beta **Cutoff:** 16.00 Å **Intensity:** Densitometer

SYS: Orthorhombic **SPGR:** Pmmm (47)
Author's Cell [AuthCell a: 7.7 Å AuthCell b: 11.95 Å AuthCell c: 5.4 Å AuthCell Vol: 496.88 Å³]
AuthCell Z: 4.00 AuthCell MolVol: 124.22 []
Author's Cell Axial Ratio [a/b: 0.701 a/c: 0.644 c/b: 0.452]
Density [Dcalc: 1.85 g/cm³ Dmeas: 1.85 g/cm³] SS:FOM: F(23) = 3.8(0.042, 141)
Temp: 298.0 K (Ambient temperature assigned by ICDD editor) Avg. Melting Point: 438 K Color: Colorless

Space Group: Pmmm (47) **Molecular Weight:** 138.36 g/mol
Crystal Data [XlCell a: 7.700 Å XlCell b: 11.950 Å XlCell c: 5.400 Å XlCell α: 90.00° XlCell β: 90.00° XlCell γ: 90.00° XlCell Vol: 496.88 Å³ XlCell Z: 4.00]
Crystal Data Axial Ratio [a/b: 0.701 a/c: 0.644 c/b: 0.452]
Reduced Cell [RedCell a: 5.400 Å RedCell b: 7.700 Å RedCell c: 11.950 Å RedCell α: 90.00° RedCell β: 90.00° RedCell γ: 90.00° RedCell Vol: 496.88 Å³]

cc: =1.412 **noβ:** =1.501 **ey:** =1.526 **Sign:** - **2θ:** =53°

Crystal (Symmetry Allowed): Centrosymmetric

Subfiles: Inorganic, Mineral Related (Mineral, Natural) **Pearson Symbol:** cP56.00 **Pearson Symbol w/o H:** cP32

Cross-Ref PDF #'s: 00-020-0669 (Primary)

References:

Type	DOI	Reference
Primary Reference		Hanawalt, J., et al. Anal. Chem. 10, 475 (1938).
Optical Data		Microscopic Character of Artificial Minerals, 2nd Ed. Cogné, Italy. Dana's System of Mineralogy, 7th Ed.
Unit Cell		

Database Comments: Color: Colorless. Deleted Or Rejected By: See 00-020-0669 (better data). General Comments: D.1 in C O2). Melting Point: 438 K. Warning: Lines with abs(delta 2Theta)>0.06 DEG.

d-Spacings (2θ) - Mg C O3 · 3 H2 O - 00-001-0130 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å

2θ(°)	d(Å)	I	h	k	l	2θ(°)	d(Å)	I	h	k	l
13.6116	6.500000	100	1	1	0	34.3302	2.610000	48	0	4	1
15.2636	5.800000	8	0	2	0	35.7431	2.510000	40	3	1	0
17.8682	4.960000	8	0	1	1	38.2680	2.350000	8	1	2	2
23.0218	3.960000	80	2	0	0	41.5029	2.170000	16	2	1	2
24.8591	3.830000	16	1	2	1	45.0670	2.010000	8	3	3	1
27.5933	3.230000	16	2	2	0	47.3049	1.920000	32	4	0	0
29.5542	3.020000	24	2	1	1	49.7851	1.830000	8	3	4	1
32.2912	2.770000	16	2	3	0	50.9763	1.790000	24	0	5	2

✓ Page setups are saved for each report type

- PDF Card
- Diffraction Patterns
- Sieve+
- etc...

✓ Page setups are saved between program sessions

1/1

1/1

2θ(°)	d(Å)	I	h	k	l	2θ(°)	d(Å)	I	h	k	l
35.5815	5.110000	16	5	3	0	20.8183	4.380000	54	0	2	5
38.0245	4.500000	54	5	1	1	48.1821	2.920000	8	3	4	1
31.8913	3.530000	16	5	3	0	41.3049	2.350000	35	4	0	0
54.9201	2.990000	16	1	5	1	42.0610	2.300000	8	3	3	1
53.0518	3.080000	80	5	0	0	41.2959	2.310000	16	5	1	5
11.9825	7.490000	0	1	1	1	28.5860	3.260000	8	1	5	2
12.3638	7.290000	0	1	5	0	32.1421	2.810000	80	2	1	0
13.6116	6.500000	100	1	1	0	34.3305	2.610000	48	0	4	1

5θ(°) q(Å) I P K I * 5θ(°) q(Å) I P K I * 5θ(°) q(Å) I P K I *