

New Features for Release 2024

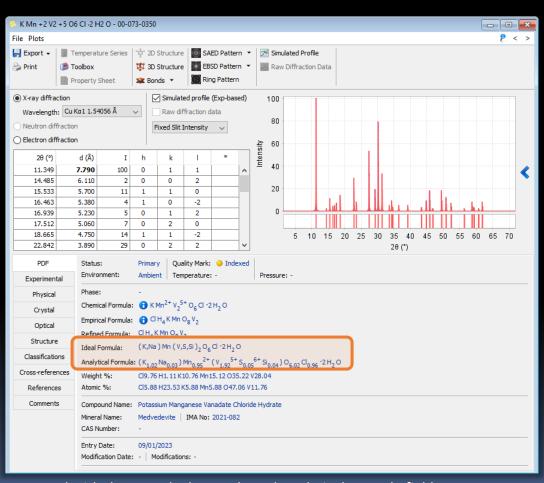
PDF-5+ 2024 Database



- PDF-4+ and PDF-4/Organics have been combined into a single database
- Contains 1,061,898 entries
- Use both sets of data simultaneously or individually



New Formula Fields



Ideal Formula

 Describes the general chemistry of the compound, especially in cases of minerals and solid solutions. Minor substituents or variations may be ignored in this representation.

Analytical Formula

 Based on experimental elemental analysis, such as XRF and microprobe analysis. This formula is descriptive and represents a composition derived based on experimental measurements.





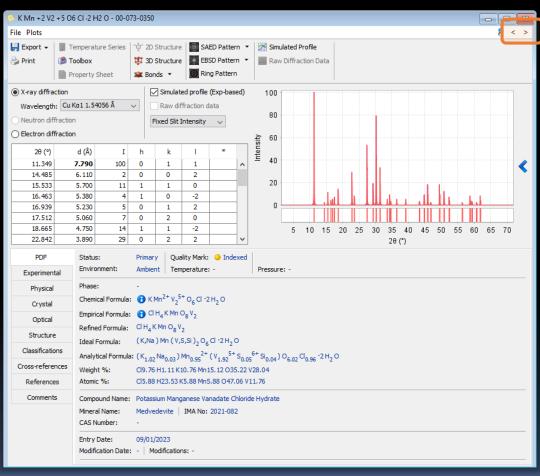
Optimized Element Searches

⊗ Search																		-	<u> </u>	X
Ş Subfile ▼					Δ	Enviror	nment		✓ Sta	atus		🌟 (Quality I	Mark		Database				
Custom PDF Set					Ambient				✓ Primary		🔑 Star - 🔑 Blank				ICDD (00)					
Alkaloid Amino Acid, Peptide & Complex				[Non-ambient				✓ Alternate		Good Low-Precision				ICSD (01)					
Battery Material					Temp. Press.				Dele	ted	↓ Indexed				CSD (02)					
				Temp. & press.						Calculated					NIST (03)					
No Subclass Depressant											Prototyping					LPF (04)				
····Narcotic					Atomic coordinates						Minimal Acceptable				ICDD Crystal Data (05)					
Pesticide & Ant	timicrob	ial	,	_ □	Raw	diffrac	tion dat	ta			~	viiriimai	Accepta	ible						
Periodic Table	ABC	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
Formula/Name	1	H Boolean O Yes/No/Maybe O Composition list He									П									
2D Structure	2	3 Li	⁴ Be	○ Ar	nd 🔘	Or	Not	Gro	uping:		4	5		5 B	⁶ C	⁷ N	o	9 F	10 Ne	
Classifications		11	12	_	nly (0	And (Or				13	14	15	.6	17	18	
Crystallography	3	Na 19	Mg		Only (B, C, N)							33	S	CI	Ar 36					
Modulated	4	~ K	Ca	21 Sc	Ti.	٧				²⁷ Co	Ni 	Cu	³⁰ Zn	"Ga	Ge	As	Se	Br	~Kr	
Diffraction	5	3/Rb	[™] Sr	39 Y	⁴⁰ Zr	⁴¹ Nb	⁴Mo		[™] Ru	Rh	[™] Pd	⁴⁄Ag	[™] Cd	‴In	Sn Sn	51 Sb	⁵≅Te	₂₃ I	S⁴Xe	
Physical Properties	6	55 Cs	⁵⁶ Ba		72 Hf	⁷³ Ta	⁷⁴ W	75 Re	76 Os		78 Pt	⁷⁹ Au	™Hg	81 TI	⁸² Pb	⁸³ Bi	⁸⁴ Po	⁸⁵ At	Rn Rn	
Reference	7	87 Fr	⁸⁸ Ra		Rf	Db	106 Sg	107 Bh	Hs Hs	109 M t	Ds	Rg	¹¹² Cn	113 Nh	114 FI	Mc	116 Lv	117 Ts	¹¹⁸ Og	
Comments					57	58	59	60	61				65					70	71	
				La:	″La	[™] Ce	⁵⁹ Pr		Pm	Sm	Eu	⁶⁴ Gd	⁶⁵ Tb	⁶⁶ Dy	Ho	⁶⁸ Er	Tm	~Yb	'Lu	
				Ac:	⁸⁹ Ac	90 Th	⁹¹ Pa	⁹² U	⁹³ Np	94 Pu	⁹⁵ Am	⁹⁶ Cm	⁹⁷ Bk	98 Cf	99 Es	Fm	Md	No No	Lr	
Range Input ▼ [Only (B, C, N)] and [Exclude deleted/hypothetical patterns]																				
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The "Only" and "Just" operators for the periodic table search have been optimized for faster results

	2023	2024
Only (B, C, N)	2.6s	0.5s
Just (H, C, N, P, O)	45.5s	7.3s
Just (Mg, B, Al, C, Si, N, O, F)	2m 38s	1s

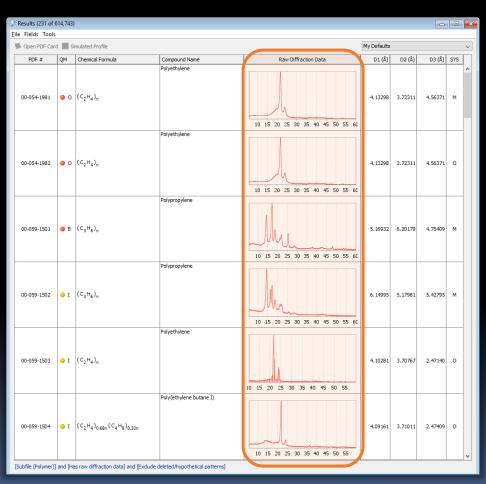
PDF Card Features



- New arrow buttons allow the user to quickly traverse through the search results table
 - Mouse wheel option



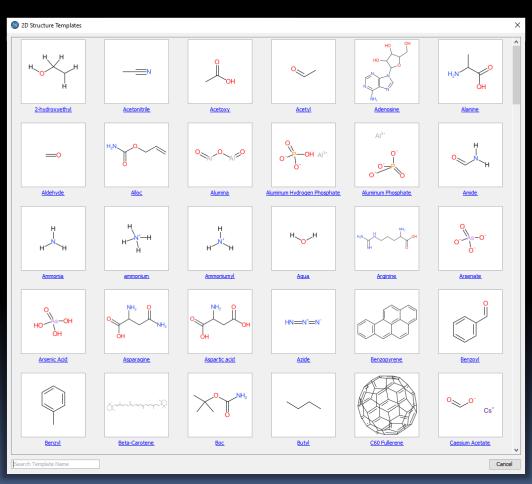
Graphing Features



- Automatic vertical zooming
- Gradient color fill option
- Raw data (PD3 patterns) in search results*
- Diffraction pattern preview when dragging and dropping*



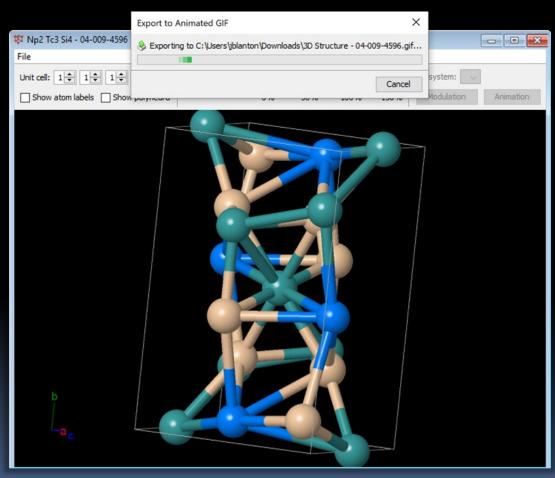
2D Structure Templates*



- Used for 2D structure and substructure searches
- 200 templates available
- Use as starting structure or complete structure
- Search by template name



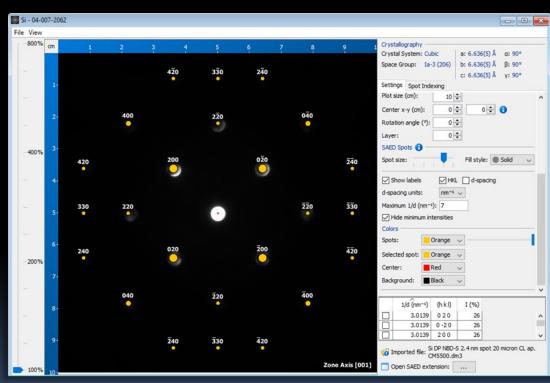
3D Structure Features*



 Export 3D structure animation to a GIF file



SAED Simulation Features*

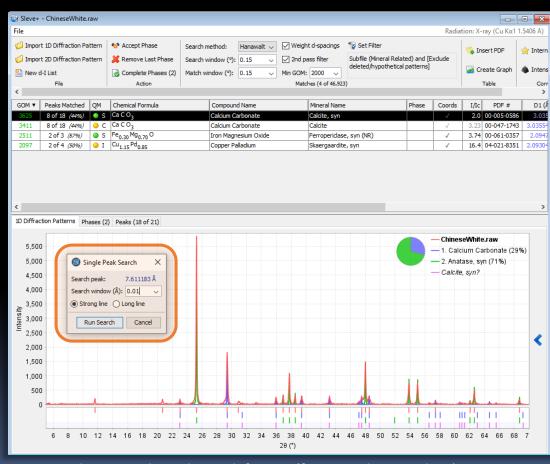


Imported Gatan *.dm3 image overlay on SAED simulation of silicon

- Added support for importing Gatan *.dm3 files
- Fill style for spots
 - Gradient
 - Solid



Sleve/Sleve+ Features

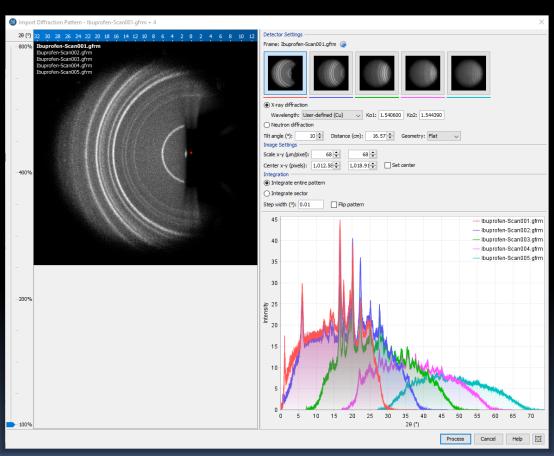


- Support for new file formats
 Rigkau *.asc
 - Rigkau *.rasx
- Hide irrelevant matches
- Supports NIST SRM 660c as an internal standard
- Single peak search
 - Select peak using the mouse
 - Search strong or long lines
 - User-defined error window
 - Useful for trace phase analysis





2D Diffraction Features*



- 2D images are dynamically displayed when importing multiple files
- Red vertical line indicates progress of pattern integration
- Thumbnail preview images



