

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

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*PDF

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

🚷 Search				
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 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 Kα1/Kα2 for removing the Kα2 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



Sleve/Sleve+ Dynamic Settings

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



Sleve/Sleve+ Features

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- 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 (20 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



Micro-XRF / Microprobe Analysis Search

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Settings																	

- "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 o	f 398,726		
le Tools Displa	y Fields: My Defaults Help		
PDF #	Chemical Formula	Compound Name	Γ
00-004-0157	C ₁₁ H ₁₇ N O ₃ ·0.5 H ₂ S O ₄ ·2 H ₂ O	Mescaline sulfate dihydrate	1
00-004-0232	C ₉ H ₁₃ N O ₃	Epinephrine	
00-005-0081	C ₁₂ H ₁₆ N ₂ O ₃	5-Ethyl-5-cyclohexenyl barbituric acid	Ī
00-005-0082	C ₂₀ H ₂₄ N ₂ O ₂	Quinidine	1
00-005-0087	C ₁₁ H ₁₈ N ₂ O ₃	Pentobarbital	Ī
00-005-0103	C ₁₀ H ₁₆ N ₂ O ₃	Butethal	1
00-005-0111	C ₈ H ₁₂ N ₂ O ₃	Barbital	Ī
00-005-0173	C ₁₂ H ₁₂ N ₂ O ₃	Phenobarbital	t
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00-005-0178	C36 H42 N2 O6 · H2 S O4 · 5 H2 O	Codeine sulfate pentahydrate	t
00-005-0179	C34 H38 N2 O6 · H2 S O4 · 5 H2 O	Morphine sulfate pentahydrate	1
00-005-0198	C ₁₂ H ₁₂ N ₂ O ₃	Phenobarbital	1
00-005-0208	C ₁₂ H ₁₂ N ₂ O ₃	Phenobarbital	1
00-005-0324	C ₁₂ H ₁₂ N ₂ O ₃	Phenobarbital	1
00-005-0345	C ₁₈ H ₂₁ N O ₃ · H ₃ P O ₄ · 2 H ₂ O	Codeine phosphate dihydrate	1
00-005-0435	H ₃ C O C ₁₁ H ₅ O ₃	Methoxsalen	1
00-006-0015	C ₁₈ H ₂₁ N O ₃ ·2 H ₂ O	Methyldihydromorphinone dihydrate	1
00-006-0016	C ₁₆ H ₂₃ N O ₂	Propylketobemidone	1
00-006-0018	C ₂₀ H ₂₃ N O ₄ · H Cl	Dihydrocodeinoneenol acetate	1
00-006-0019	C ₁₈ H ₁₉ N O ₃ · H Cl	Morphothebaine hydrochloride	Ī
00-006-0023	C ₂₄ H ₂₅ N O ₃ · H Cl	Benzylmorphine hydrochloride	Ť
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Formulas use subscripts and superscripts for proper notation and readability

- Chemical Formula
- Empirical Formula
- Structural Formula



Printing Reports

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	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 Å ² AuthOcell Z: 4.00 AuthCell MolVol: 124.22] AuthOcell Axial Ratio [Cala: 0.701 alb: 0.644 clb: 0.452] Density [Decl: 1.65 g/cm ² Dmess: 1.85 g/cm ²] SSIFOM: F(23) = 3.8(0.042, 141) Temp: 299.0 K (Ambient temperature assigned by ICDD editor) Avg. Metting Point: 438 K Color: Cldriess	
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- Page setups are saved for each report type
 - PDF Card
 - Diffraction Patterns
 - Sleve+
 - etc...
- Page setups are saved between program sessions