

PDF-4

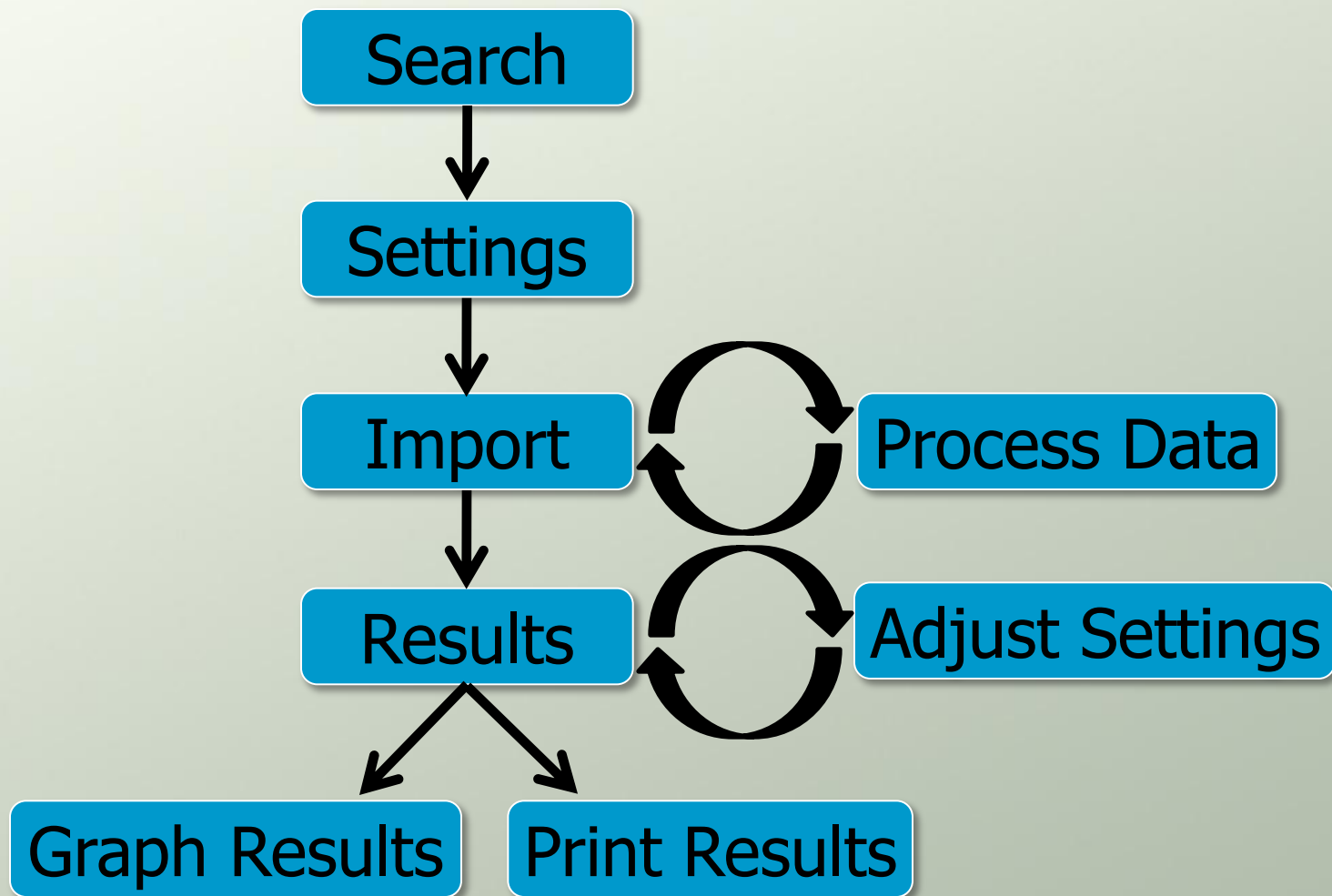
Integral Index

A similarity index for comparing diffraction patterns

What is the Integral Index?

- The Integral Index creates numerical values based on the user's full experimental data compared to patterns in the PDF-4+ database. These index values can then be used as an additional tool for data mining and trend analysis.
- The Integral Index formula is a sum of the differences between the full experimental pattern and a simulated full pattern. The simulated full pattern is calculated from the database using instrumental and experimental factors. This formula is based on the Hofmann and Kuleshova similarity index.
- The Integral Index value ranges from 0-100%. The lower the index value, the better the match, giving 0% a perfect match and 100% a complete non-match.

The Integral Index Process



Search

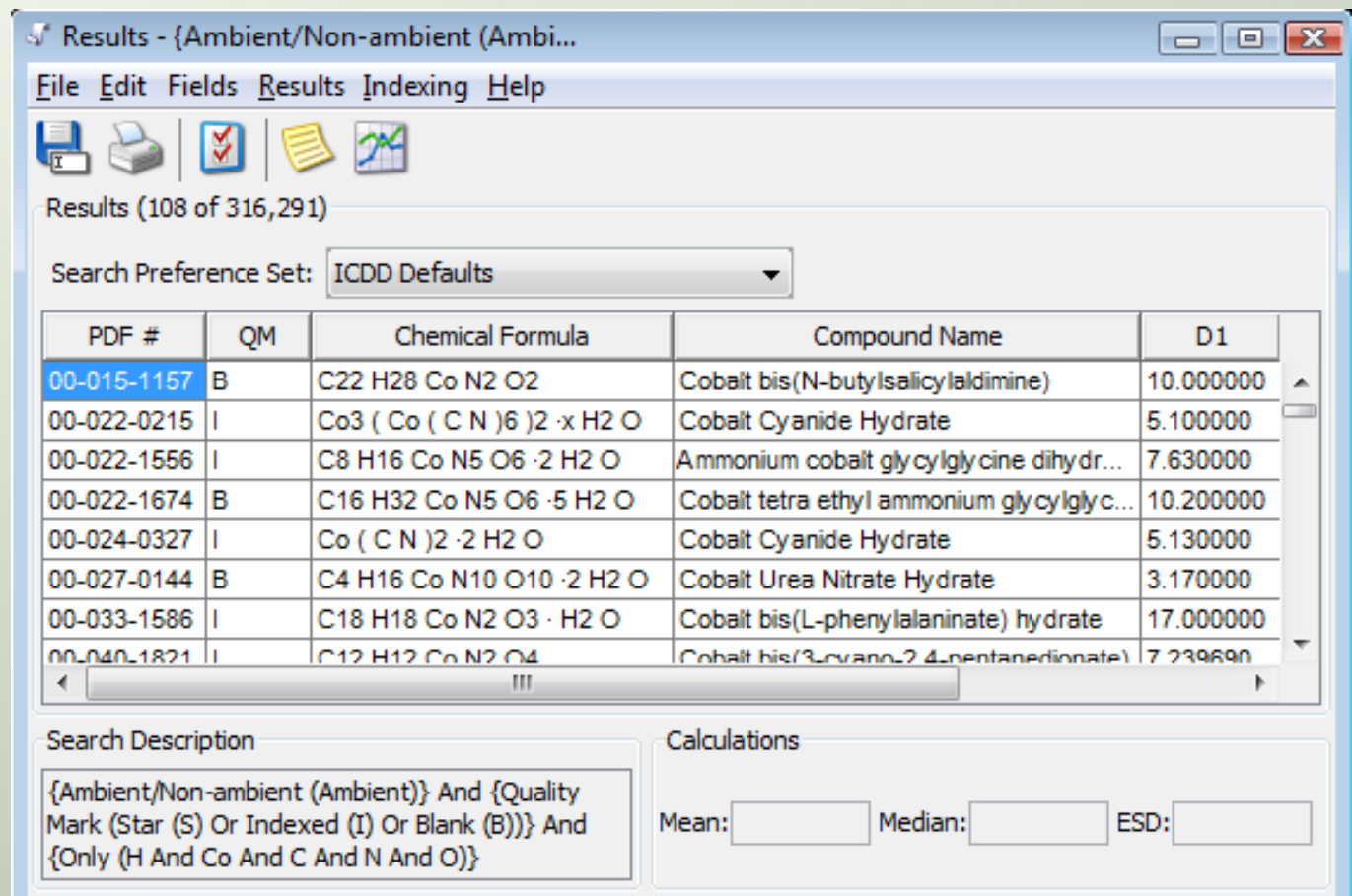
The first step in utilizing the Integral Index method is to create search criteria based on non-whole pattern data. This effectively narrows down the entire database into a more meaningful form.

Search Criteria:

- Only Cobalt, Hydrogen, Nitrogen, Oxygen, & Carbon
- Ambient
- Quality Mark Star Or Indexed Or Blank

Search Results

- After a search is performed, the results window will automatically appear.



Results - {Ambient/Non-ambient (Ambi...}

File Edit Fields Results Indexing Help

Results (108 of 316,291)

Search Preference Set: ICDD Defaults

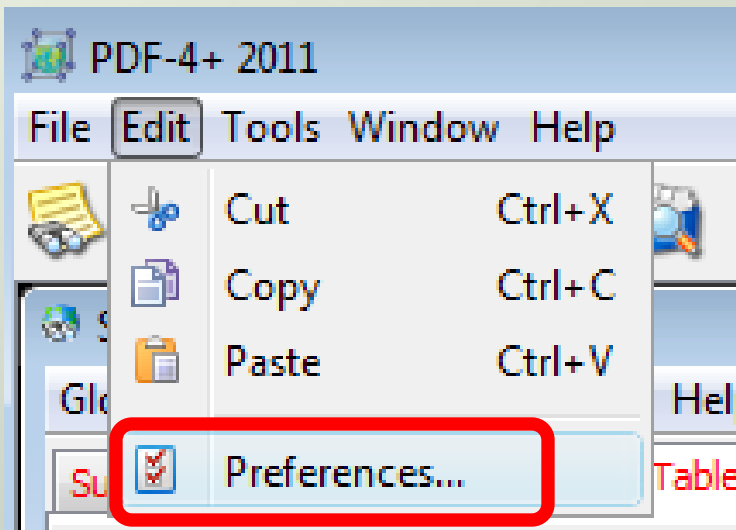
PDF #	QM	Chemical Formula	Compound Name	D1
00-015-1157	B	C ₂₂ H ₂₈ Co N ₂ O ₂	Cobalt bis(N-butylsalicylaldimine)	10.000000
00-022-0215	I	Co ₃ (Co (C N) ₆) ₂ · x H ₂ O	Cobalt Cyanide Hydrate	5.100000
00-022-1556	I	C ₈ H ₁₆ Co N ₅ O ₆ · 2 H ₂ O	Ammonium cobalt glycyglycine dihydr...	7.630000
00-022-1674	B	C ₁₆ H ₃₂ Co N ₅ O ₆ · 5 H ₂ O	Cobalt tetra ethyl ammonium glycyglyc...	10.200000
00-024-0327	I	Co (C N) ₂ · 2 H ₂ O	Cobalt Cyanide Hydrate	5.130000
00-027-0144	B	C ₄ H ₁₆ Co N ₁₀ O ₁₀ · 2 H ₂ O	Cobalt Urea Nitrate Hydrate	3.170000
00-033-1586	I	C ₁₈ H ₁₈ Co N ₂ O ₃ · H ₂ O	Cobalt bis(L-phenylalaninate) hydrate	17.000000
00-040-1821	I	C ₁₂ H ₁₂ Co N ₂ O ₄	Cobalt bis(3-oxo-2,4-pentanedionate)	7.239690

Search Description: {Ambient/Non-ambient (Ambient)} And {Quality Mark (Star (S) Or Indexed (I) Or Blank (B))} And {Only (H And Co And C And N And O)}

Calculations: Mean: Median: ESD:

Set Preferences

- Before you import full experimental data, you must change the diffraction graph settings to match.
- Select preferences in the main menu or click the double-check icon on the main toolbar.



Diffraction Graph Preferences

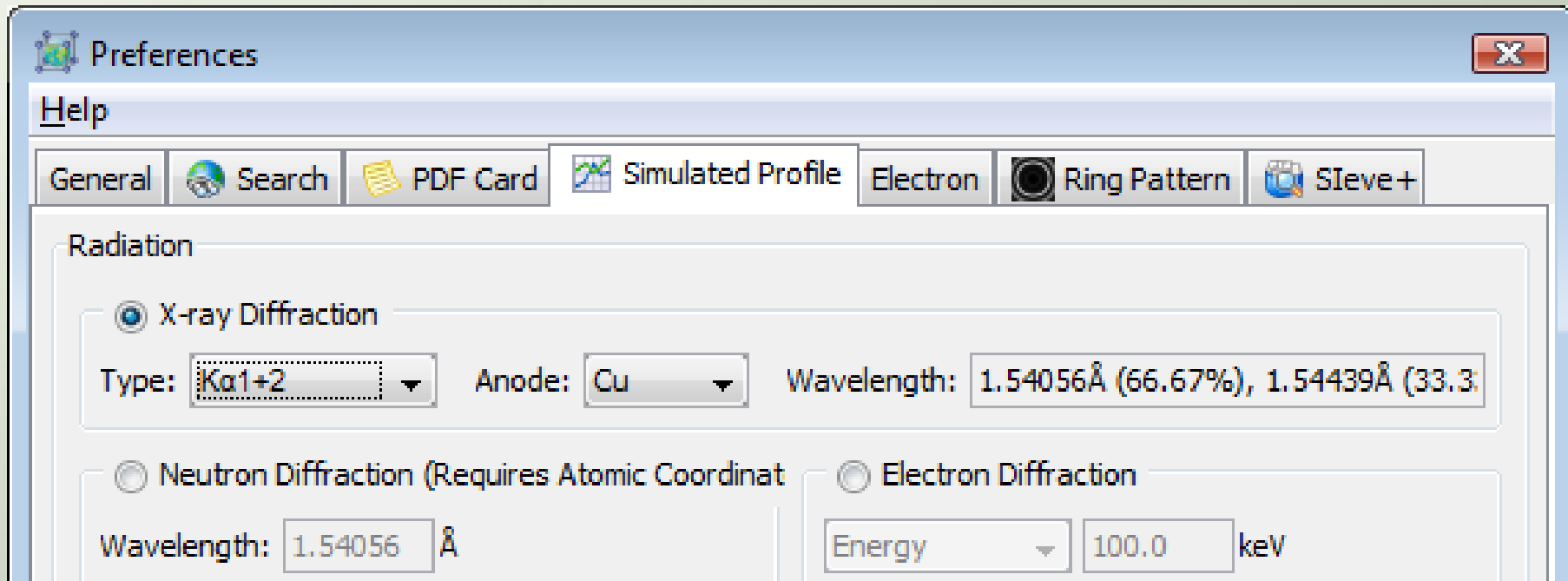
- There are 2 sets of preferences for diffraction graphs: experimental and calculated.
- Calculated patterns have either structure factors or atomic coordinates in the database.
- The diffraction graph will specify calculated or experimental on the form.

PDF-4+ 2011	Calculated	Experimental
ICDD	4,528	102,469
ICSD-FIZ	0	60,633
NIST	0	3,297
LPF	145,364	0

Experimental Diffraction Preferences

Under “Edit” >> “Preferences” on the menu
Select the “Simulated Profile” tab.

Adjust the settings to match the experiment.



Preferences

Help

General Search PDF Card Simulated Profile Electron Ring Pattern Sieve +

Radiation

X-ray Diffraction

Type: Anode: Wavelength:

Neutron Diffraction (Requires Atomic Coordinates)

Wavelength: Å

Electron Diffraction

Energy: keV

Calculated Diffraction Preferences

- Go lower down on the Simulated Profile tab.
- Adjust the settings to match the experiment.

Geometry (Calculated Patterns Only)

Bragg-Brentano: Fixed Slit Polarization Fraction: 0.0 Sample Thickness: 0.1 mm
 Debye Scherrer

Profile

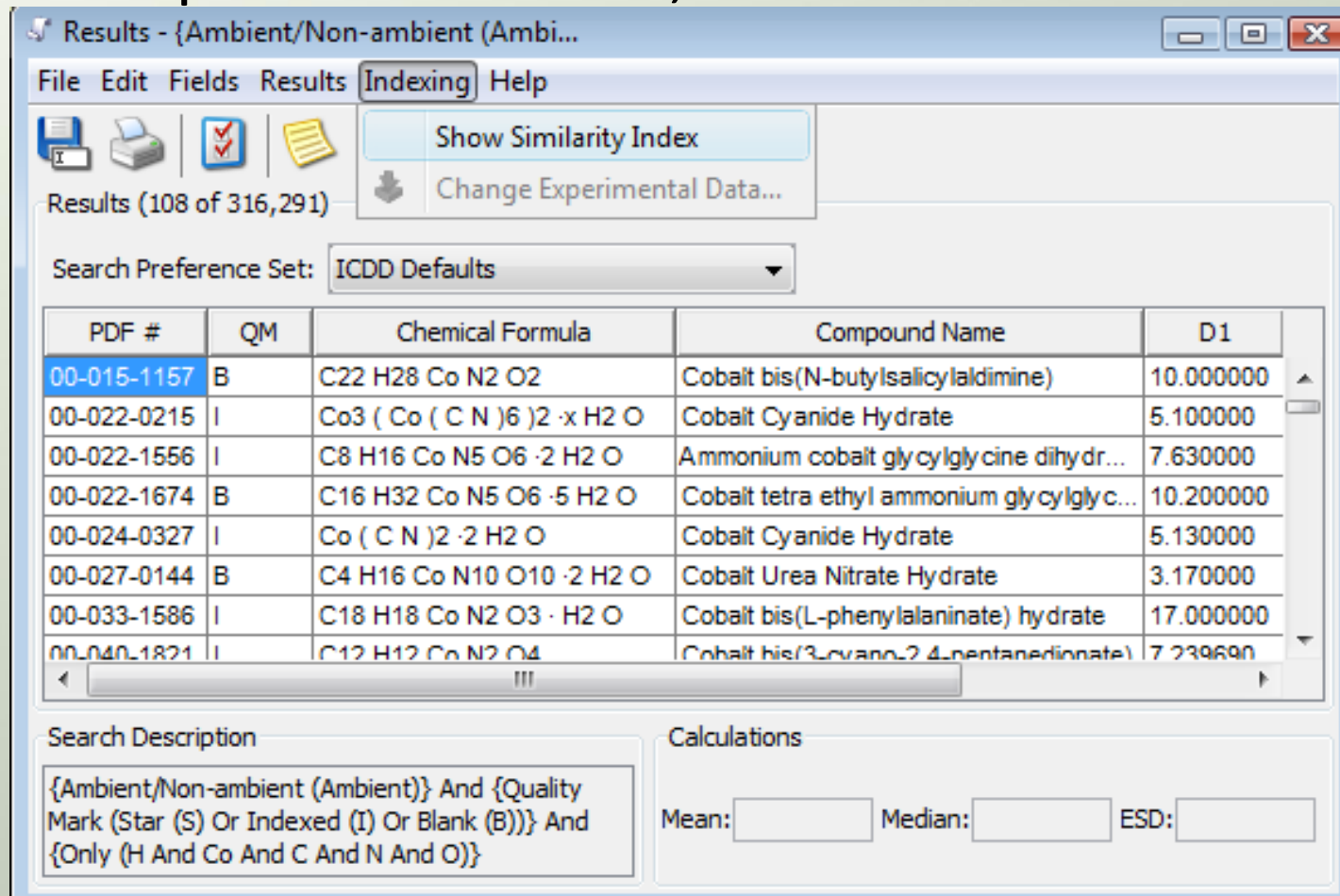
Pseudo-Voigt U: 0.002717 V: -0.00076 W: 0.003636 A: 0.8 B: 0.0
Significance Limit: 0.01

Range

- The range and step size are automatically set for the Integral Index from the whole pattern experimental data and cannot be changed by the Diffraction Preferences.

Import Data

- On the results form, select “Show Similarity Index” under “Indexing”, or “Change Experimental Data”, if it is enabled.



Results - {Ambient/Non-ambient (Ambi...}

File Edit Fields Results **Indexing** Help

Results (108 of 316,291)

Search Preference Set: ICDD Defaults

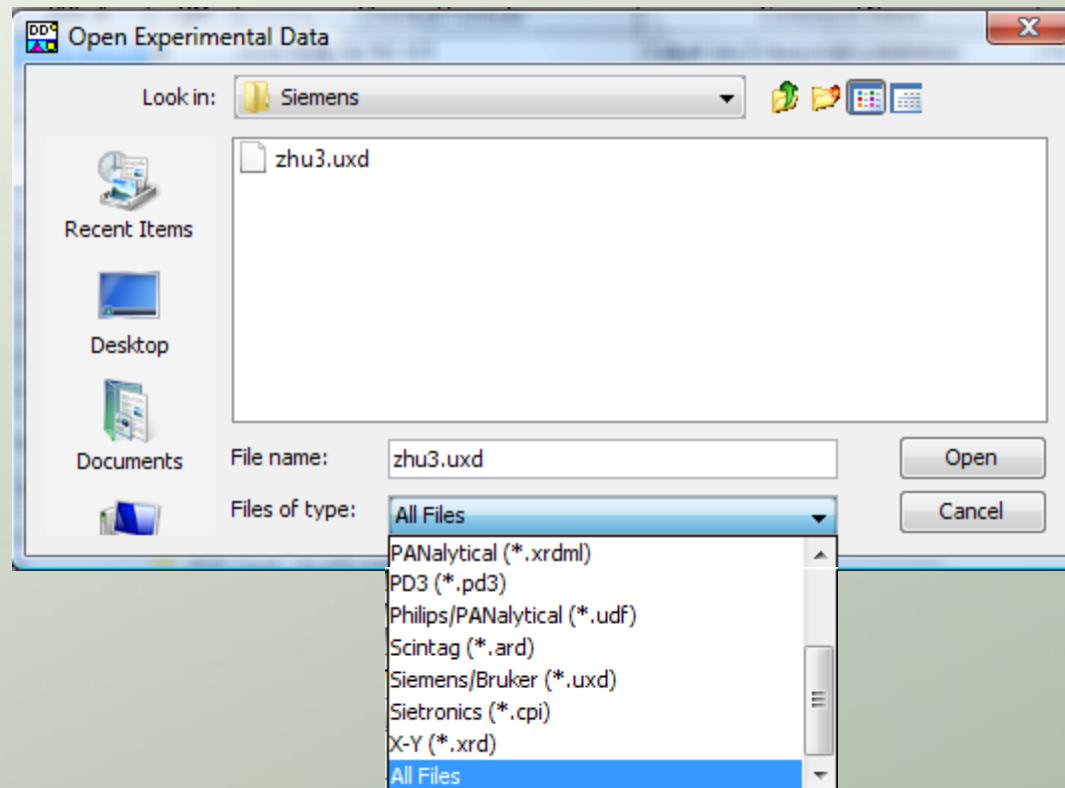
PDF #	QM	Chemical Formula	Compound Name	D1
00-015-1157	B	C22 H28 Co N2 O2	Cobalt bis(N-butylsalicylaldimine)	10.000000
00-022-0215	I	Co3 (Co (C N)6)2 ·x H2 O	Cobalt Cyanide Hydrate	5.100000
00-022-1556	I	C8 H16 Co N5 O6 ·2 H2 O	Ammonium cobalt glycyglycine dihydr...	7.630000
00-022-1674	B	C16 H32 Co N5 O6 ·5 H2 O	Cobalt tetra ethyl ammonium glycyglyc...	10.200000
00-024-0327	I	Co (C N)2 ·2 H2 O	Cobalt Cyanide Hydrate	5.130000
00-027-0144	B	C4 H16 Co N10 O10 ·2 H2 O	Cobalt Urea Nitrate Hydrate	3.170000
00-033-1586	I	C18 H18 Co N2 O3 · H2 O	Cobalt bis(L-phenylalaninate) hydrate	17.000000
00-040-1821	I	C12 H12 Co N2 O4	Cobalt bis(3-Oxano-2,4-pentanedionate)	7.239690

Search Description: {Ambient/Non-ambient (Ambient)} And {Quality Mark (Star (S) Or Indexed (I) Or Blank (B))} And {Only (H And Co And C And N And O)}

Calculations: Mean: Median: ESD:

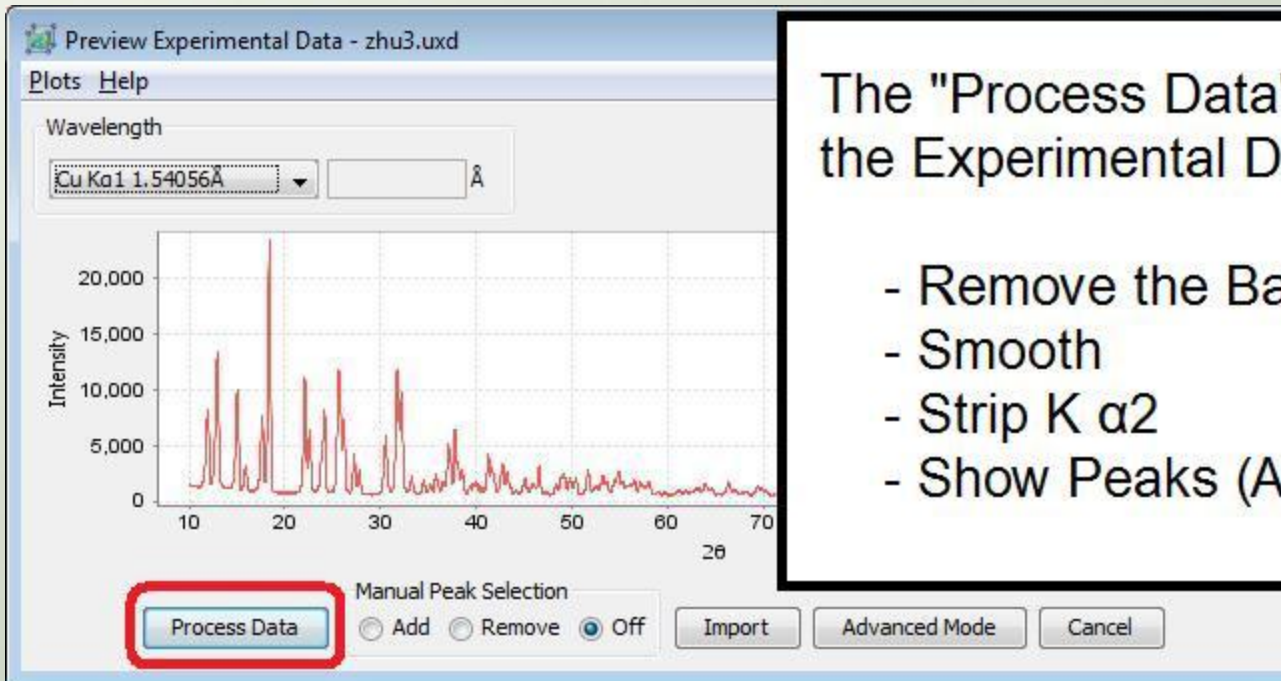
Selecting a File

- You can import a number of different file formats supporting various diffractometers and software.



Processing the Imported Data

Since database patterns have been processed to eliminate background, noise and $K\alpha_2$ peaks, the same needs to be done to the experimental data to identify peaks.

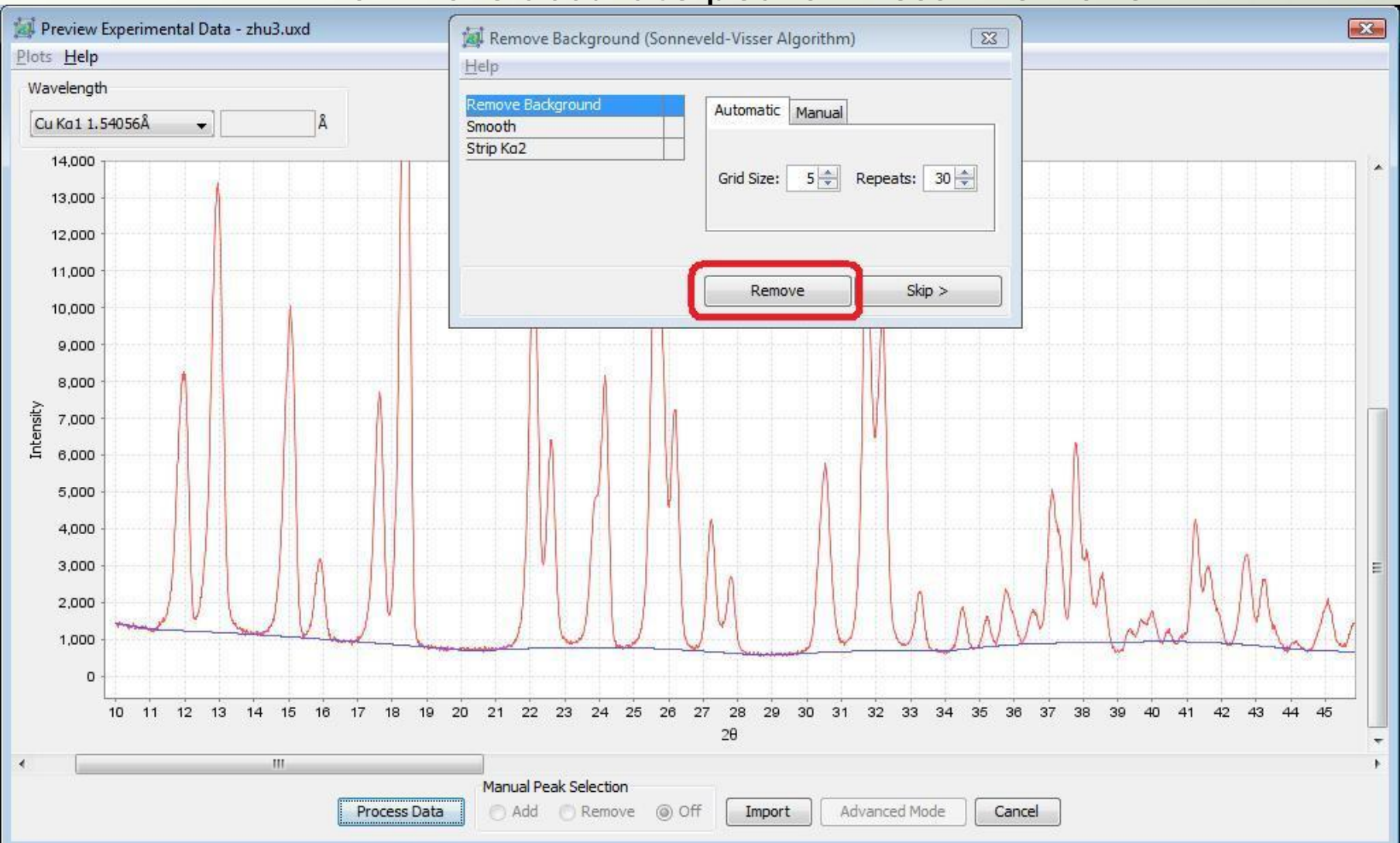


The "Process Data" button will process the Experimental Data so as to:

- Remove the Background
- Smooth
- Strip $K\alpha_2$
- Show Peaks (Automatically)

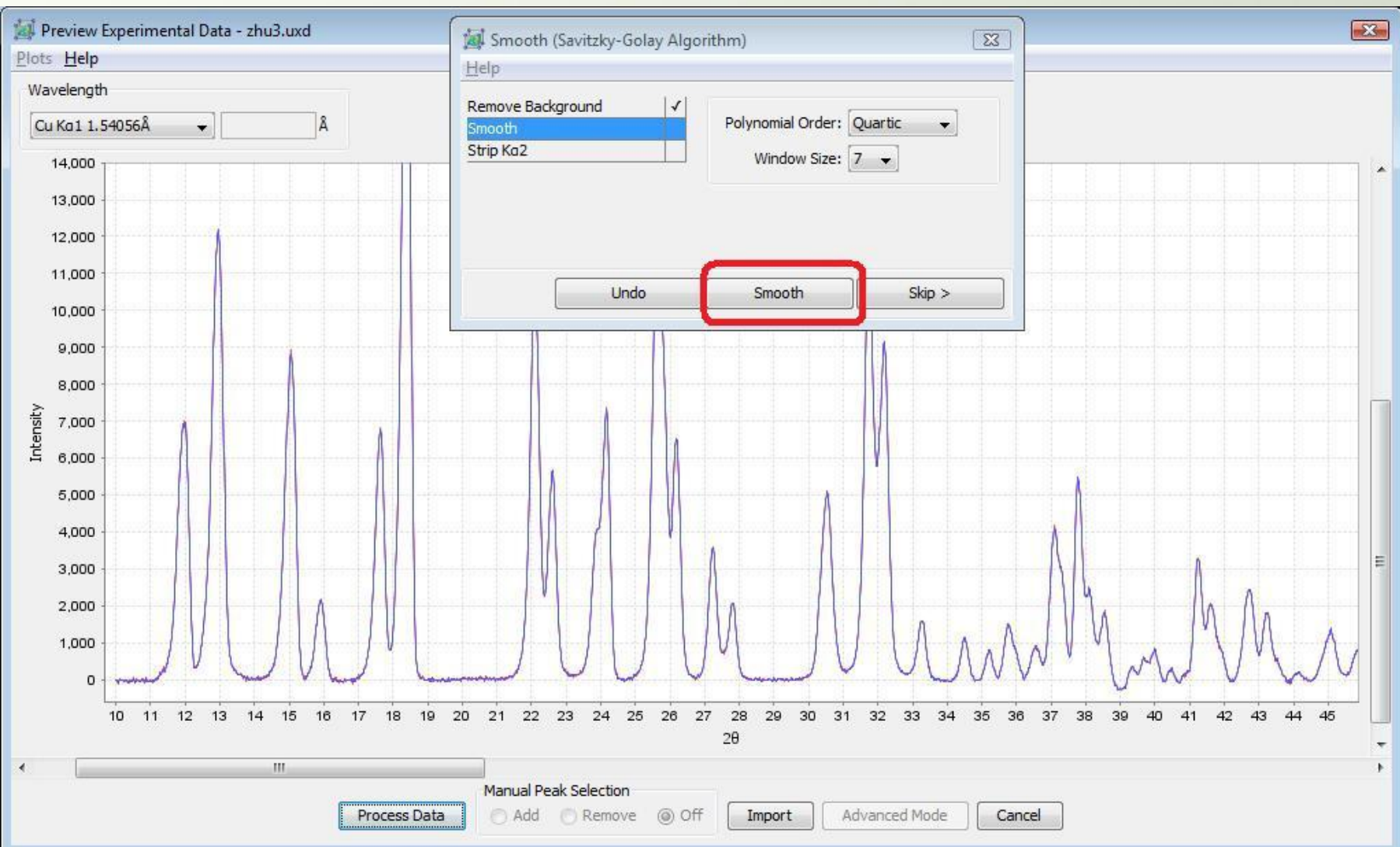
Removing the Background

Remove background noise and air scatter for more accurate peaks. Press “Remove”.



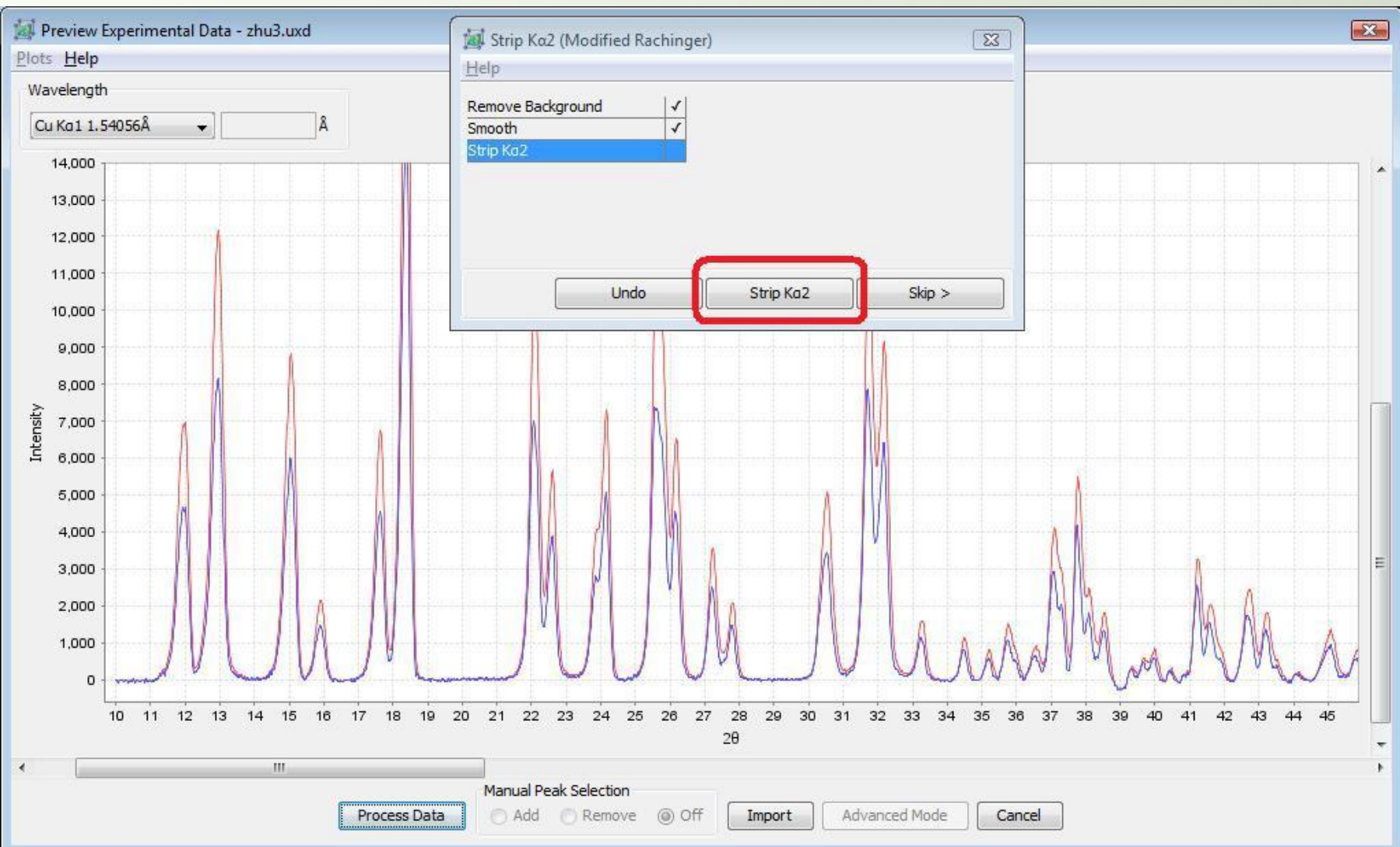
Smoothing

Note the effects of the Background removal. Now Smooth noisy patterns for consistent results and press “Smooth”.



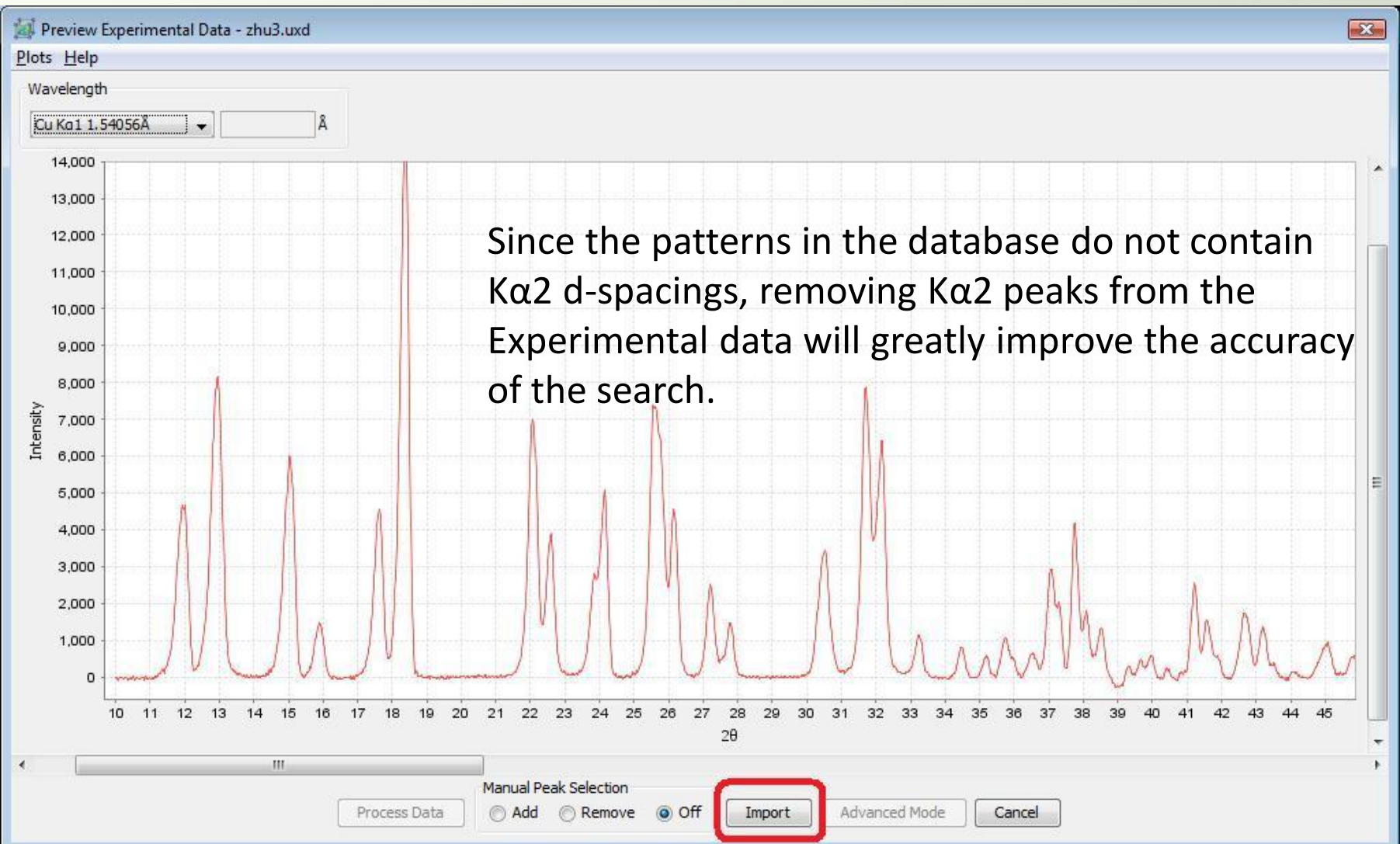
Strip $K\alpha_2$

Note the effects of the Smoothing. Now press “Strip $K\alpha_2$ ”.



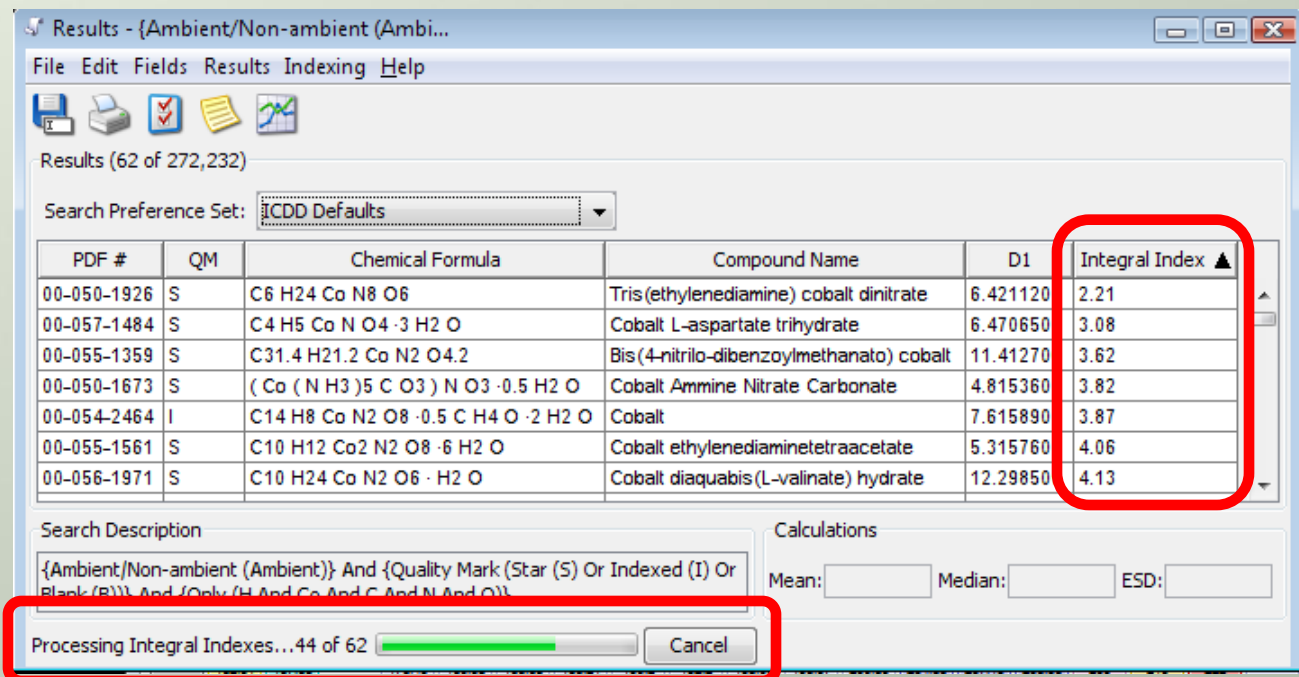
Import

Finally, press “Import” to run the Index calculations.



Integral Index Display

- The Integral Index is added to the right side of the results form. Lowest value is the best match.
- After it is completed, the status in the lower left corner will disappear.
- Clicking on the column title will sort it.



Results - {Ambient/Non-ambient (Ambi...}

File Edit Fields Results Indexing Help

Results (62 of 272,232)

Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name	D1	Integral Index ▲
00-050-1926	S	C6 H24 Co N8 O6	Tris(ethylenediamine) cobalt dinitrate	6.421120	2.21
00-057-1484	S	C4 H5 Co N O4 · 3 H2 O	Cobalt L-aspartate trihydrate	6.470650	3.08
00-055-1359	S	C31.4 H21.2 Co N2 O4.2	Bis(4-nitrilo-dibenzoyl-methanato) cobalt	11.41270	3.62
00-050-1673	S	(Co (N H3) 5 C O3) N O3 · 0.5 H2 O	Cobalt Ammine Nitrate Carbonate	4.815360	3.82
00-054-2464	I	C14 H8 Co N2 O8 · 0.5 C H4 O · 2 H2 O	Cobalt	7.615890	3.87
00-055-1561	S	C10 H12 Co2 N2 O8 · 6 H2 O	Cobalt ethylenediaminetetraacetate	5.315760	4.06
00-056-1971	S	C10 H24 Co N2 O6 · H2 O	Cobalt diaquabis(L-valinate) hydrate	12.29850	4.13

Search Description: {Ambient/Non-ambient (Ambient)} And {Quality Mark (Star (S) Or Indexed (I) Or Black (B))} And {Only (H And Co And C And N And O)}

Calculations: Mean: [] Median: [] ESD: []

Processing Integral Indexes... 44 of 62 [Progress Bar] Cancel

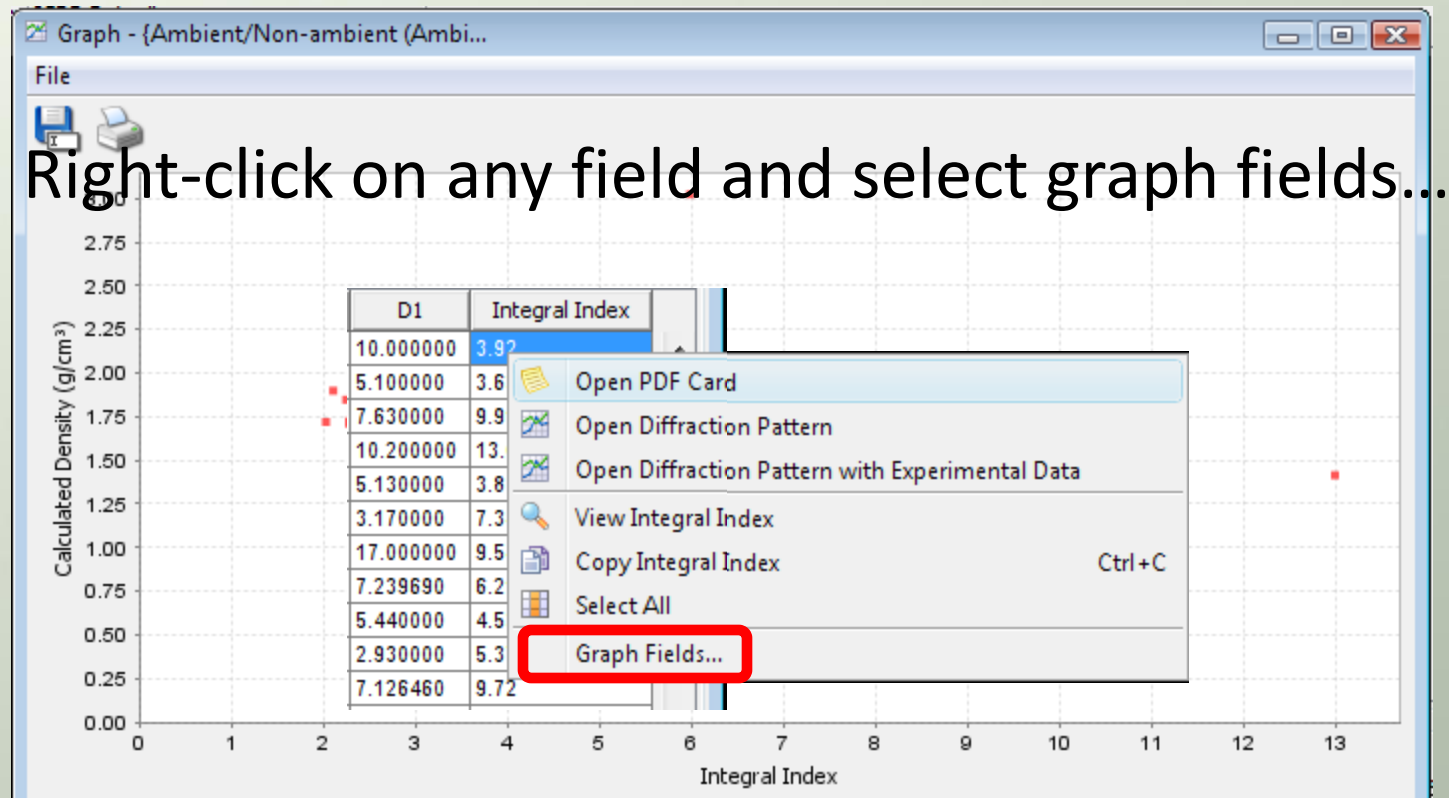
Using the Data

Get the most out of the data by using other tools and features

- **Histogram** – Plot the Integral Index against any database field or the number of results.
- **Print a report** – Create a customized report on your results using any database fields on any size paper.
- **Plot a graph** – Overlay a simulated full pattern of any database entry with your experimental data.

Histogram

Compare sets of data to determine patterns and attributes of your results.



Report

Print a report using the menu on the results form or click on the printer icon.

zhu3.uxd Results - Print Preview

File Navigation Zoom Help

100 %

Aug 27, 2007 10:58 AM (crane)

zhu3.uxd Results

Description: {Ambient/Non-ambient (Ambient)} And {Quality Mark (Star (S) Or Indexed (I) Or Blank (B))} And {Only (H And Co And C And N And O)}

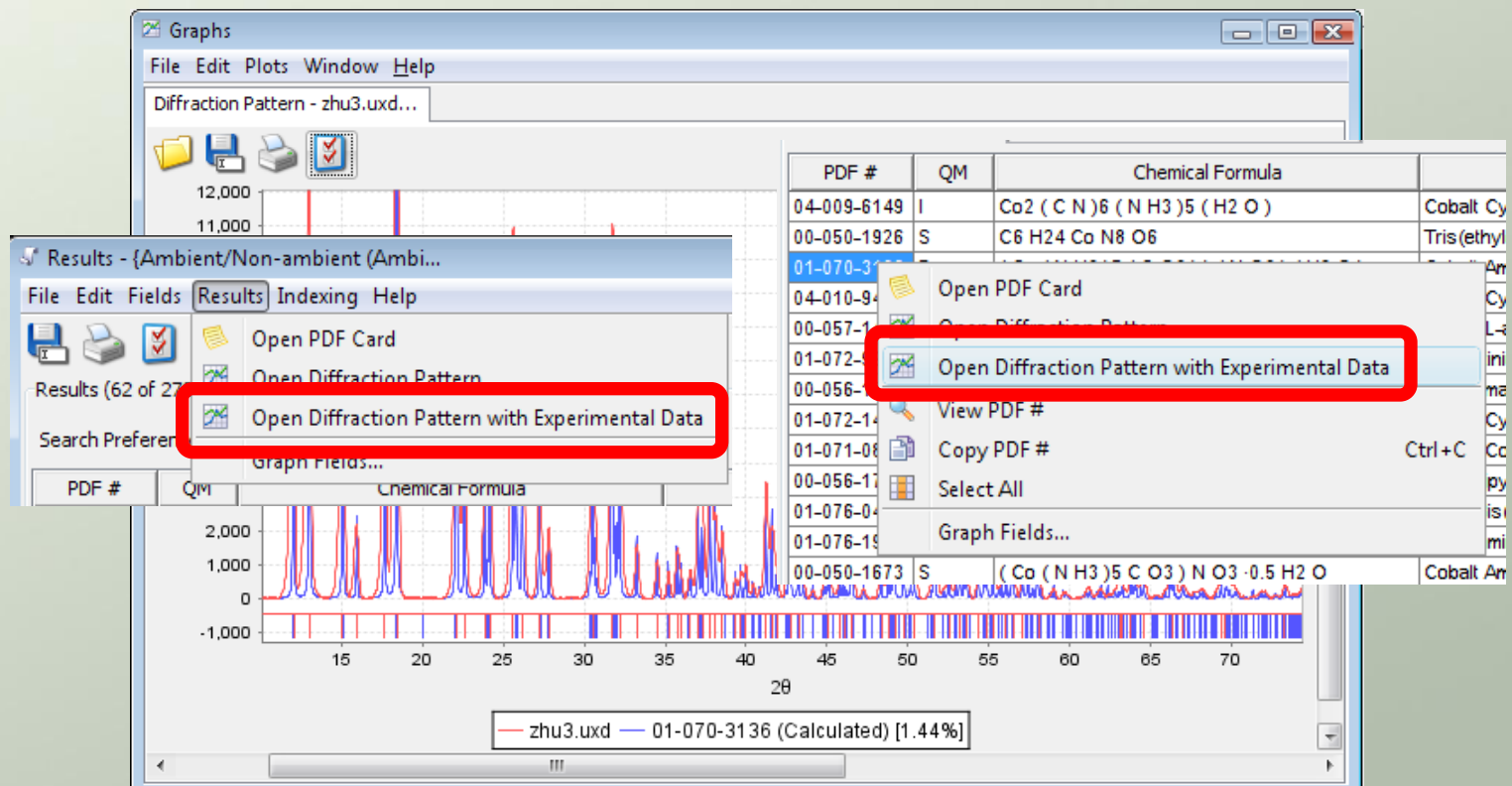
PDF #	QM	Chemical Formula	Compound Name	D1	Integral Index
04-009-6149	I	Co ₂ (C N) ₆ (N H ₃) ₅ (H ₂ O)	Cobalt Cyanide Amine Hydrate	4.965540	2.07
00-050-1926	S	C ₆ H ₂₄ Co N ₈ O ₆	Tris(ethylenediamine) cobalt dinitrate	6.421120	2.56
01-070-3136	B	(Co (N H ₃) ₅ (C O ₃) (N O ₃) (H ₂ O)	Cobalt Ammine Carbonate Nitrate Hydrate	4.820000	2.15
04-010-9448	S	Co ₂ (C N) ₆ (N H ₃) ₅ (H ₂ O)	Cobalt Cyanide Ammine Hydrate	4.962720	2.32
00-057-1484	S	C ₄ H ₅ Co N O ₄ · 3 H ₂ O	Cobalt L-aspartate trihydrate	6.470650	2.5
01-072-9989	B	(N ₂ H ₅) (Co (N H N H ₂ C O O) ₃) (H ₂ O)	Hydrazinium tris(hydrazidocarbonato)cobaltate hydrate	4.621890	2.39
00-056-1875	S	C ₁₅ H ₁₀ Co N ₂ O ₄ · 2 H ₂ O	Cobalt malonate (1,10-phenanthroline) dihydrate	6.799330	2.32
01-072-1431	B	(Co ₃ (Co (C N) ₆) ₂ (H ₂ O) ₁₂) _{1.3333}	Cobalt Cyanide Hydrate	5.105000	2.52
01-071-0807	B	(Co ₃ (Co (C N) ₆) ₂ (H ₂ O) ₁₂) _{1.333}	Cobalt Cobalt Cyanide Hydrate	5.105000	2.52
00-056-1754	S	C ₂₄ H ₁₄ Co ₂ N ₄ O ₈ · 7 H ₂ O	(4,4'-Bipyridyl)bis(2,6-pyridinedicarboxylato) cobalt heptahydrate	6.000920	2.52
01-076-0476	B	Co (N O ₂) ₂ (C ₂ H ₄ (N H ₂) ₂) ₂ N O ₃	trans-Bis(ethylenediamine) dinitrocobalt nitrate	6.491170	2.56
01-076-1955	B	Co (O C O N H ₂) (N H ₃) ₅ (N O ₃) ₂	Pentamminecarbamato cobalt nitrate	6.222580	2.73
00-050-1673	S	(Co (N H ₃) ₅ (C O ₃) N O ₃ · 0.5 H ₂ O	Cobalt Ammine Nitrate Carbonate Hydrate	4.815360	2.29
00-055-1359	S	C _{31.4} H _{21.2} Co N ₂ O _{4.2}	Bis(4-nitro-dibenzoyl-methanato) cobalt ethanol clathrate	11.412700	2.67
01-072-0826	B	(Co ₃ (C N) ₂ (O H) ₄ (N H ₃) ₈) (Co ₂ (N O ₂) ₆ (O H) ₂ N O ₂) H ₂ O)	Dicyanocobalt-Tetra-μ-Hydroxo-Bis(Tetraammine)cobalt Di-μ-Hydroxo-μ-Nitro-Bis(Trinitrocobaltate)	5.939800	2.85

Page 1 of 3

Graph

Using the results form menu, or by right clicking on an entry, you can display a graph overlaying the selected pattern over the experimental pattern.

Determine the experiment's range and set the range accordingly to correctly display diffraction graphs.



Thank you for viewing our tutorial.
Additional tutorials are available at the ICDD website:
www.icdd.com

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