

Combine Searches

Save Time with
The History Form

The History Form

What?

For a given session, a list of past searches is automatically saved each time a search is run. This list can be found in the History form.

More complex searches, not possible by running Search alone, can be obtained by combining past searches in the History form.

The History Form

Why?

By selecting various criteria to develop a simple or complex search, you can search the entire database or limit the data examined.

By saving this information, alternative searches can be compared for precision and efficiency.

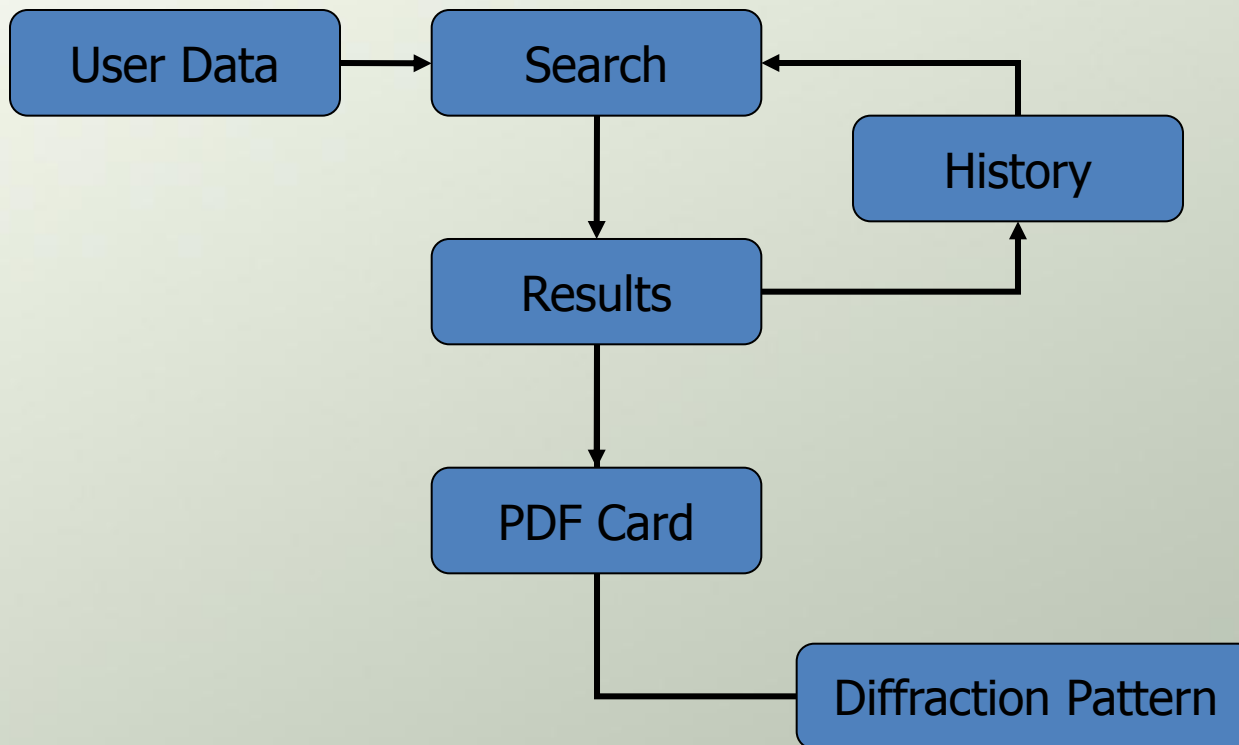
Advanced Searches

How?

A Criteria History or “History” form is provided to record and display the selected criteria. Each criteria listed is followed by the number of matches.

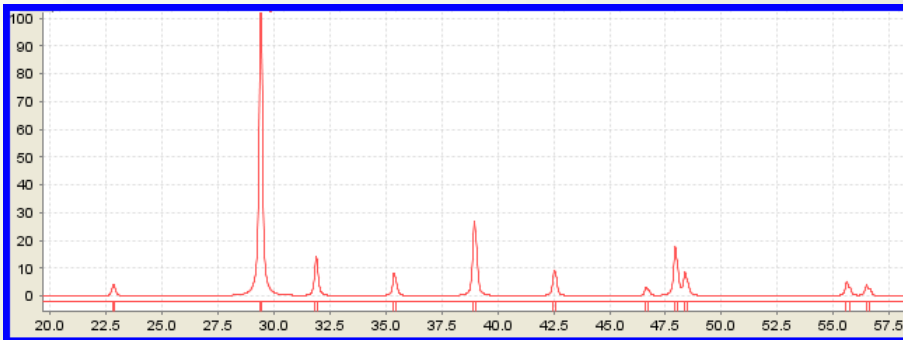
You have the option of viewing the Search Result, examining a specific PDF entry, further refining your search parameters, or saving the Criteria History in a file for retrieval at another time.

The Data Mining Process



Illustrative Example

A bottle is labeled NaNO3. Is it?



You obtain an X-ray diffractogram at 4 degrees 2θ per minute and read rough 2θ 's and I's.

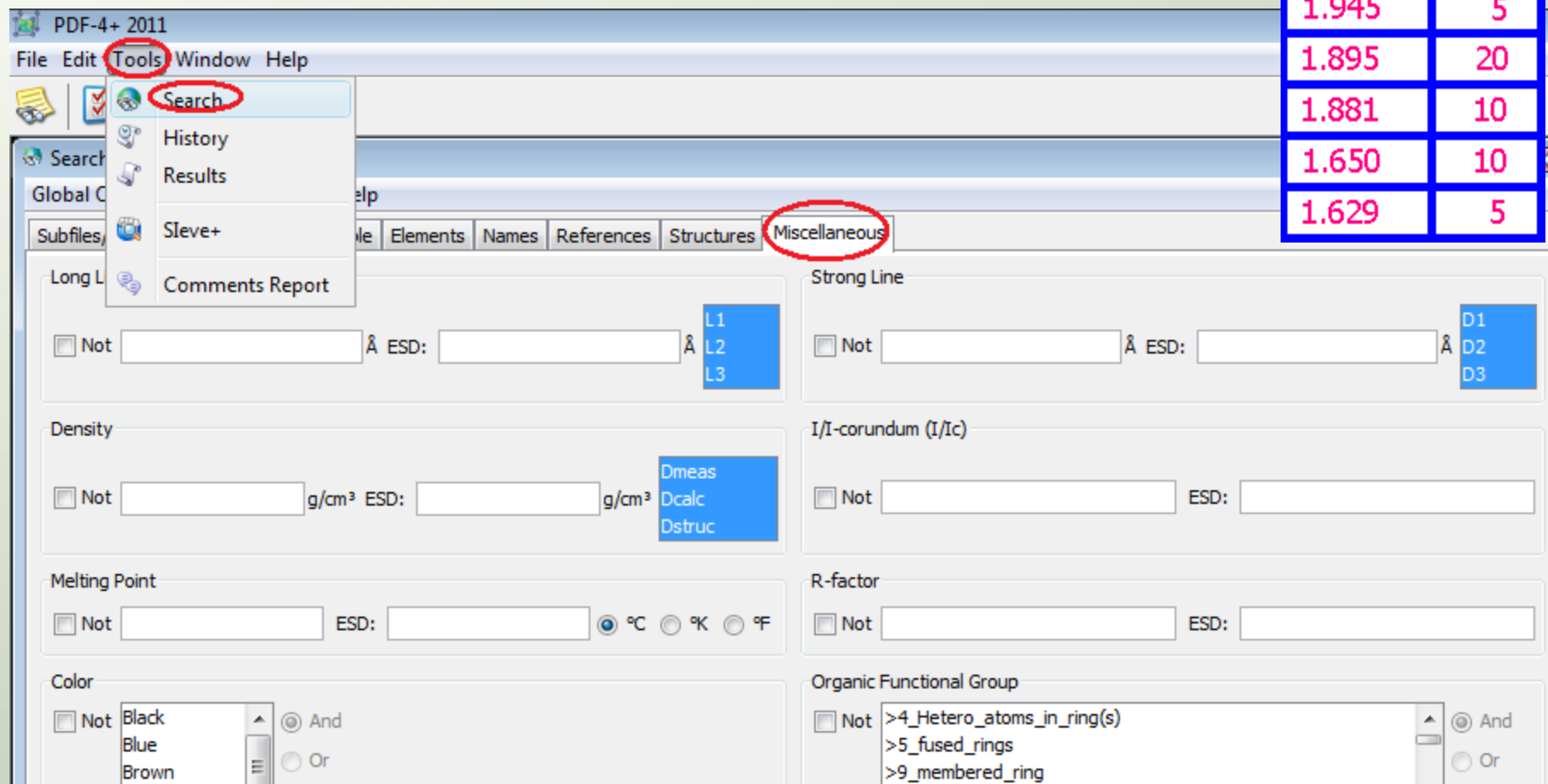
You convert the 2θ 's into d-spacings (Angstroms), using Bragg's Law. ($\lambda = 1.54056$, K α Copper).

Use History to find compounds in the database which match your experiment.

$2\theta^\circ$ (Cu K α)	d(Å)	Int
22.9	3.88	10
29.4	3.04	100
32.0	2.797	20
35.4	2.536	10
39.0	2.309	20
42.6	2.122	15
46.7	1.945	5
48.0	1.895	20
48.4	1.881	10
55.7	1.650	10
56.5	1.629	5

d(Å)	Int
3.88	10
3.04	100
2.797	20
2.536	10
2.309	20
2.122	15
1.945	5
1.895	20
1.881	10
1.650	10
1.629	5

To use History, we first must have a Search in RAM. Go to Tools >> Search>> Miscellaneous tab



The screenshot shows the PDF-4+ 2011 software interface. The 'Tools' menu is open, with 'Search' highlighted. The 'Miscellaneous' tab is selected in the search criteria area. The interface includes various search filters such as 'Strong Line', 'Density', 'Melting Point', 'R-factor', and 'Organic Functional Group'. The 'Miscellaneous' tab is circled in red, and the 'Search' menu item is also circled in red.

Your strongest line is 3.04A. Enter this into the textbox (1), and specify plus or minus .08A (2). Then click Search (3) and the Results will appear, showing all phases in the database with any of the 3 strongest lines in the range of 3.04 - .08 to 3.04 + .08 (4). We now have this search in RAM, so History knows about it. We can now Reset the Page and do another Search (5). The Reset Page button does not remove this search from RAM or History. It only clears the Search Window.

$d(\text{\AA})$	Int
3.88	10
3.04	100
2.797	20
2.536	10
2.309	20
2.122	15
1.945	5
1.895	20
1.881	10
1.650	10
1.629	5

PDF-4+ 2011

File Edit Tools Window Help



Miscellaneous

Strong Line **1** **2**

Not 3.04 Å ESD: .08 Å

I/I-corundum (I/Ic)

Not _____ ESD: _____

R-factor

Not _____ ESD: _____

Organic Functional Group

Not >4_Hetero_atoms_in_ring(s)
>5_fused_rings
>9_membered_ring
1_Hetero_atom_in_ring(s)
1,2_dione___O=C-C=O

3 **5**

Search Show Result Undock Page

4 Results - {Strong Line = 3.04(.08)Å}...

File Edit Fields Results Indexing Help

Results (60,304 of 316,291)

Search Preference Set: ICDD Defaults

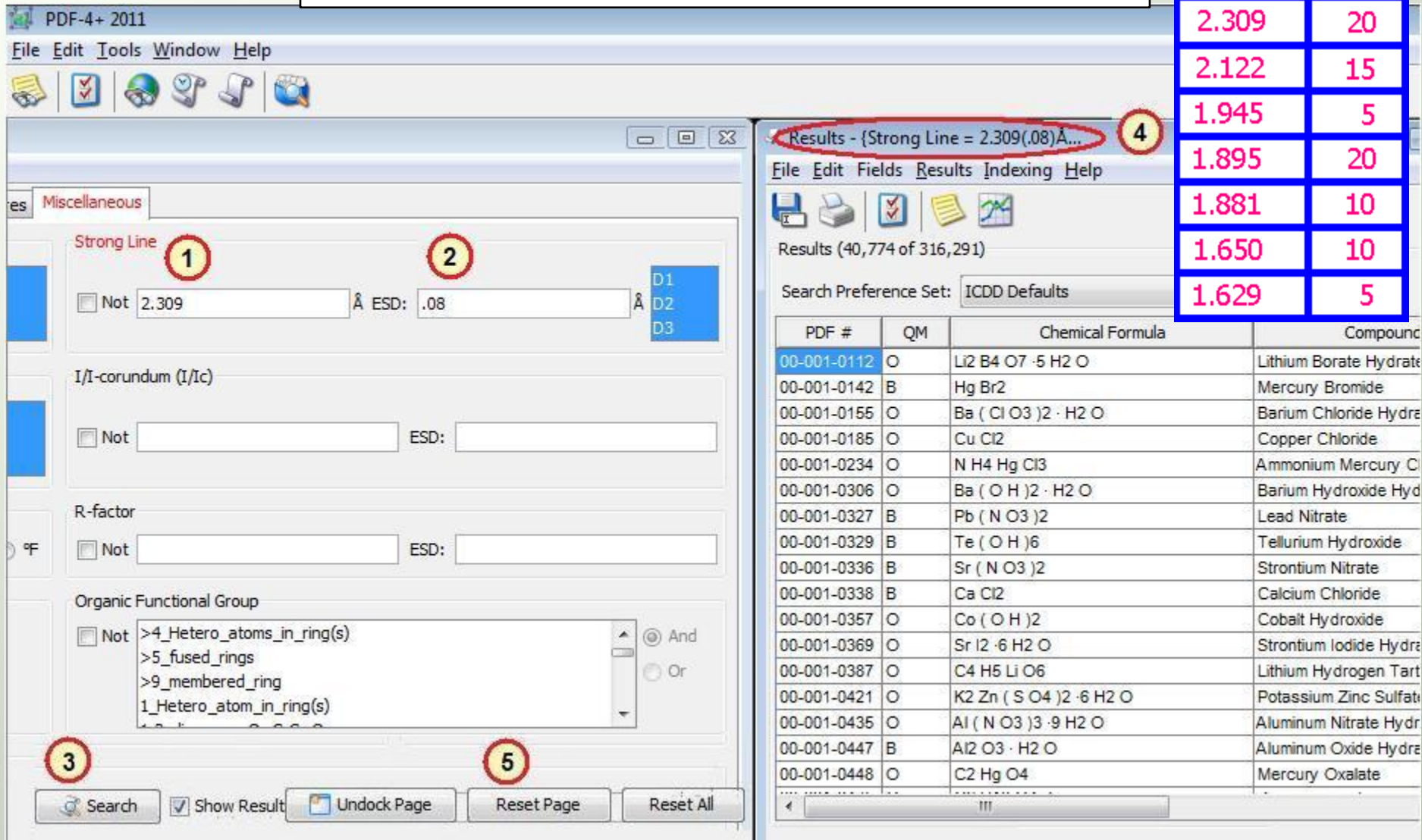
PDF #	QM	Chemical Formula	Compound
00-001-0008	O	C12 H10 Ca3 O14 · 4 H2 O	Calcium citrate hydrat
00-001-0020	O	C6 H4 H O O C C O O K	Potassium hydrogen F
00-001-0023	O	Pb (C2 H3 O2)2 · Pb (O H)2 · H2 O	Lead Hydrate Acetate
00-001-0040	O	(N H4)2 W O4 · x H2 O	Ammonium Tungsten (
00-001-0046	O	C21 H15 Bi O6	Bismuth benzoate
00-001-0048	O	C8 H12 Ca2 O12 · 7 H2 O	Calcium gly colate hep
00-001-0049	O	Ag C2 H3 O2	Silver Acetate
00-001-0050	O	Na C2 H3 O2	Sodium Acetate
00-001-0051	O	Cu (C2 H3 O2)2 · 3 Cu (As O2)2	Copper Acetate Arser
00-001-0053	O	C14 H10 Ca O6 · 3 H2 O	Calcium salicylate trity
00-001-0054	O	Cu3 (P O4)2 · 3 H2 O	Copper Phosphate Hy
00-001-0065	O	Ba (C2 H3 O2)2 · H2 O	Barium Acetate Hydra
00-001-0067	O	Mg Pt (C N)6	Magnesium Platinum C
00-001-0070	O	Au K (C N)2	Gold Potassium Cyani
00-001-0113	O	Na2 Mo O4 · 2 H2 O	Sodium Molybdenum H

Search Description: {Strong Line = 3.04(.08)Å}

Calculations: Mean: _____ Median: _____ ESD: _____

Your second strongest line is 2.309A. Enter this into the textbox (1), and specify plus or minus .08A (2). Then click Search (3) and the Results will appear, showing all phases in the database with any of the 3 strongest lines in the range of 2.309 - .08 to 2.309 + .08. (4). Now that we have this search in RAM, History has it in its list. We can click on the Reset Page button and do another search (5).

$d(\text{\AA})$	Int
3.88	10
3.04	100
2.797	20
2.536	10
2.309	20
2.122	15
1.945	5
1.895	20
1.881	10
1.650	10
1.629	5



The screenshot shows the PDF-4+ 2011 software interface. The 'Miscellaneous' tab is active. The 'Strong Line' section has '2.309' entered in the 'Not' field (1) and '.08' in the 'ESD' field (2). The 'Search' button (3) is highlighted. The 'Results' window shows a list of search results with the title 'Results - {Strong Line = 2.309(.08)Å...' (4). The results table is as follows:

PDF #	QM	Chemical Formula	Compound
00-001-0112	O	Li2 B4 O7 · 5 H2 O	Lithium Borate Hydrate
00-001-0142	B	Hg Br2	Mercury Bromide
00-001-0155	O	Ba (Cl O3)2 · H2 O	Barium Chloride Hydrate
00-001-0185	O	Cu Cl2	Copper Chloride
00-001-0234	O	N H4 Hg Cl3	Ammonium Mercury Chloride
00-001-0306	O	Ba (O H)2 · H2 O	Barium Hydroxide Hydrate
00-001-0327	B	Pb (N O3)2	Lead Nitrate
00-001-0329	B	Te (O H)6	Tellurium Hydroxide
00-001-0336	B	Sr (N O3)2	Strontium Nitrate
00-001-0338	B	Ca Cl2	Calcium Chloride
00-001-0357	O	Co (O H)2	Cobalt Hydroxide
00-001-0369	O	Sr I2 · 6 H2 O	Strontium Iodide Hydrate
00-001-0387	O	C4 H5 Li O6	Lithium Hydrogen Tartarate
00-001-0421	O	K2 Zn (S O4)2 · 6 H2 O	Potassium Zinc Sulfate Hydrate
00-001-0435	O	Al (N O3)3 · 9 H2 O	Aluminum Nitrate Hydrate
00-001-0447	B	Al2 O3 · H2 O	Aluminum Oxide Hydrate
00-001-0448	O	C2 Hg O4	Mercury Oxalate

The 'Organic Functional Group' section is also visible, with '>4_Hetero_atoms_in_ring(s)' selected. The 'Reset Page' button (5) is highlighted at the bottom.

Your third strongest line is 1.895Å. Enter this into the textbox (1) and specify plus or minus .08Å (2). Then click on the Search button (3) and the results will appear, showing all phases in the database with any of the 3 strongest lines in the range of 1.895 - .08Å to 1.895 + .08Å. (4). Click on the Reset Page button and we will do one more search (5).

$d(\text{Å})$	Int
3.88	10
3.04	100
2.797	20
2.536	10
2.309	20
2.122	15
1.945	5
1.895	20
1.881	10
1.650	10
1.629	5

PDF-4+ 2011
File Edit Tools Window Help

Miscellaneous

Strong Line **1** **2**

Not 1.895 Å ESD: .08 Å

I/I-corundum (I/Ic)

Not ESD:

R-factor

Not ESD:

Organic Functional Group

Not >4_Hetero_atoms_in_ring(s) And
>5_fused_rings Or
>9_membered_ring
1_Hetero_atom_in_ring(s)

Has PD3 Pattern Yes No

Has Property Sheet Yes No

3 Search Show Results Undock Page **5** Reset Page Reset All

4 Results - (Strong Line = 1.895(.08)Å...

File Edit Fields Results Indexing Help

Results (39, 152 of 316, 291)

Search Preference Set: ICDD Defaults


PDF #	QM	Chemical Formula	Phase Name
00-001-0172	B	Mn Cl2	Manganese(II) Chloride
00-001-0206	O	Cu S C N	Copper Thiocyanate
00-001-0239	O	Fe4 (Fe (C N)6)3	Iron Cyanide
00-001-0265	I	Al2 O3 · 3 H2 O	Aluminum Oxide Hydrate
00-001-0304	O	(N H4)2 Cu F4 · 2 H2 O	Ammonium Copper Fluoride
00-001-0356	O	Na4 P2 O7	Sodium Phosphate
00-001-0420	B	Hg2 Cl2	Mercury Chloride
00-001-0453	O	C H Ca Na O P	Sodium calcium glycerophosphate
00-001-0482	I	Ca Si F6	Calcium Silicon Fluoride
00-001-0490	O	Ti O F2	Titanium Fluoride Oxide
00-001-0495	O	Be S O4	Beryllium Sulfate
00-001-0502	O	Ag I	Silver Iodide
00-001-0503	B	Ag I	Silver Iodide
00-001-0505	O	K H2 P O4	Potassium Hydrogen Phosphate
00-001-0516	I	Ca Cr O4	Calcium Chromium Oxide
00-001-0519	B	B P O4	Boron Phosphate Oxide
00-001-0533	I	Ba F2	Barium Fluoride
00-001-0534	O	Ba Si F6	Barium Silicon Fluoride
00-001-0538	I	Sb2 S3	Antimony Sulfide
00-001-0557	I	Sn I4	Tin Iodide

Your longest line is 3.88Å. Enter this into the Long Line textbox. (1) All our other lines were entered into the Strong Line textbox. Specify plus or minus .08Å (2). Then click on the Search button (3). The Results will appear showing all phases of the database with any of the 3 longest lines in the range of 3.88 - .08Å to 3.88 + .08Å (4). We are now have four searches stored in RAM, which are ready to be used by History.

$d(\text{Å})$	Int
3.88	10
3.04	100
2.797	20
2.536	10
2.309	20
2.122	15
1.945	5
1.895	20
1.881	10
1.650	10
1.629	5

PDF-4+ 2011

File Edit Tools Window Help



Search

Global Operator Numeric Input Help

Subfiles/Database Filters Periodic Table Elements Names References Structures Mis

Long Line **1** **2**

Not 3.88 Å ESD: .08 Å

Density

Not g/cm³ ESD: g/cm³

Melting Point

Not ESD: °C °K °F

Color

Not Black Blue Brown Color Missing

Smith-Snyder Figure Of Merit (SS/FOM)

Not ESD:

3 **5**

Search Show Results Undock Page Reset Page

4

Results - {Long Line = 3.88(.08)Å}

File Edit Fields Results Indexing Help

Results (33,756 of 316,291)

Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula
00-001-0008	O	C12 H10 Ca3 O14 ·4 H2 O
00-001-0021	O	C2 H3 Hg O2
00-001-0049	O	Ag C2 H3 O2
00-001-0117	O	Te O2
00-001-0136	O	Fe +3 O (O H)
00-001-0148	O	Na3 Co (N O2)6
00-001-0181	O	Fe (H2 P O2)3
00-001-0183	O	Zn H P O3
00-001-0202	O	Fe F3 ·3 H2 O
00-001-0203	O	Al F3 ·3 H2 O
00-001-0222	O	Na B O3 ·2 H2 O
00-001-0235	O	Sb Br3
00-001-0258	O	Co F2 ·4 H2 O
00-001-0268	I	K2 Os O4 ·2 H2 O
00-001-0272	O	Na2 Se O4
00-001-0283	O	C2 Mn O4 ·2 H2 O
00-001-0290	O	N H4 H S O4
00-001-0292	B	C2 Fe O4 ·2 H2 O
00-001-0294	O	C6 H12 N2 O4
00-001-0295	O	C2 O4 Zn ·2 H2 O

History

File Help

Past Searches

Name	Description	Hits
Search #1	{Strong Line = 3.04(.08)Å}	60,304
Search #2	{Strong Line = 2.309(.08)Å}	40,774
Search #3	{Strong Line = 1.895(.08)Å}	39,152
Search #4	{Long Line = 3.88(.08)Å}	33,756

▼ **4**

▼ **5**

Combined Searches

Name	Description

Operation

And Or

Combined Results

Add to Past Searches

To bring up the History Form, click on Tools >> History. We can see our four searches were stored in the Past Searches History List. We could bring back the 60,304 phases which have a Strong Line of 3.04A by clicking on the Results button (1). The blue background color indicates that Search #1 is currently selected. We can select any of the four searches with the mouse, or select two or more of them by pressing the Control key and selecting with the mouse. We can rename the currently selected search by clicking on the Rename button (2). We can delete one search at a time by selecting it and clicking Delete (3). We can combine searches one by one by selecting them and clicking on button 4, or combine all four at once by clicking on button 5. Since we want a combination of our four lines, we will click on button 5.

PDF-4+ 2011

File Edit Tools Window Help

History

File Help

1

Past Searches

Name	Descri
Search #2	{Strong Line = 2.309(.08)Å}
Search #3	{Strong Line = 1.895(.08)Å}
Search #4	{Long Line = 3.88(.08)Å}

2

4

5

3

6

7

Combined Searches (56)

Name	Operation
Search #1	{Strong Line = 3.04(.08)Å}
Search #2	{Strong Line = 2.309(.08)Å}
Search #3	{Strong Line = 1.895(.08)Å}
Search #4	{Long Line = 3.88(.08)Å}

Results

Rename...

Delete

Delete All

And Or

Combined Results

Add to Past Searches

Delete

Delete All

Once we press Button 5, the Bottom part of History activates. Our 4 searches are copied from the Past Searches List (1) to the Combined Searches List (2).

Note the Operation control (3). The “AND” operator is selected by default, but we could have combined our 4 searches with any permutation of “AND” and “OR”, by adding them one by one using Button 4 instead of Button 5.

As it is, our Combined Search is:
Search#1 AND Search#2 AND Search#3 AND Search #4.

When you press Button 6, you will do two things:
Firstly, you will run the Combined Search and bring up the Results Window.
Secondly, because option 7 is checked, you will put this Search into the Top List.

Why do you want your combined Search in the top list?
Because only the Searches in the top list can be saved to a File. The information in the bottom list is only a temporary “scratch pad” in memory with which you can assemble elements from the top list. You will be able to retrieve the top list after you save it, however.

Now click Button 6.

Click on the Combined Results Button. You will see the Results Window (1) and read the Search Description (2). Note that Search#5 is now in the "Past Searches" List (3).

You want to know if your sample is Sodium Nitrate. So you double click on PDF# 01-077-6301 To bring up the PDF card (4).

PDF-4+ 2011

File Edit Tools Window Help

History

File Help

Past Searches

Name	Descri
Search #1 {Strong Line = 3.04(.08)Å}	60,304
Search #2 {Strong Line = 2.309(.08)Å}	40,774
Search #3 {Strong Line = 1.895(.08)Å}	39,152
Search #4 {Long Line = 3.88(.08)Å}	33,756
Search #5 {Strong Line = 3.04(.08)Å} And {Strong Line = 2.309(.08)Å} And {Strong Line = 1.895(.08)Å} And	56

3

Combined Searches (56)

Name	Operation
Search #1 {Strong Line = 3.04(.08)Å}	<input checked="" type="radio"/> And <input type="radio"/> Or
Search #2 {Strong Line = 2.309(.08)Å}	<input type="radio"/> Combined Results
Search #3 {Strong Line = 1.895(.08)Å}	<input checked="" type="checkbox"/> Add to Past Searches
Search #4 {Long Line = 3.88(.08)Å}	<input type="checkbox"/> Delete

Results - {Strong Line = 3.04(.08)Å}...

File Edit Fields Results Indexing Help

Results (56 of 316,291) 1

Search Preference Set: ICDD Defaults

PDF #	Chemical Formula	Compound Na
01-077-6301	Na (N O3)	Sodium Nitrate
01-078-3262	Ca (C O3)	Calcium Carbonate
01-078-4614	Ca (C O3)	Calcium Carbonate
01-079-2056	Na N O3	Sodium Nitrate
01-083-1762	Ca (C O3)	Calcium Carbonate
01-085-0849	Ca (C O3)	Calcium Carbonate
01-085-0850	Na (N O3)	Sodium Nitrate
01-085-1464	Na (N O3)	Sodium Nitrate
01-086-2334	Ca (C O3)	Calcium Carbonate
01-086-2336	(Mg.129 Ca.871) (C O3)	Magnesium Calcium Carb
01-089-2828	Na (N O3)	Sodium Nitrate
04-001-7249	Ca (C O3)	Calcium Carbonate
04-002-7275	Na (N O3)	Sodium Nitrate
04-006-9073	Na (N O3)	Sodium Nitrate
04-006-9074	Na0.85 Ag0.15 (N O3)	Sodium Silver Nitrate

4

Search Description

{Strong Line = 3.04(.08)Å} And {Strong Line = 2.309(.08)Å} And {Strong Line = 1.895(.08)Å} And {Long Line = 3.88(.08)Å}

Calculations

Mean: Median: ESD:

2

You compare the d's and I's from your experiment with the d's and I's from card # 01-077-6301, and conclude that the sample was indeed Sodium Nitrate. But now you want to save your search...

Na (N O3) - 01-077-6301

File Edit d-Spacings Tools Window Help

Wavelength: Cu Kα1 1.54056Å

Stick Patterns:

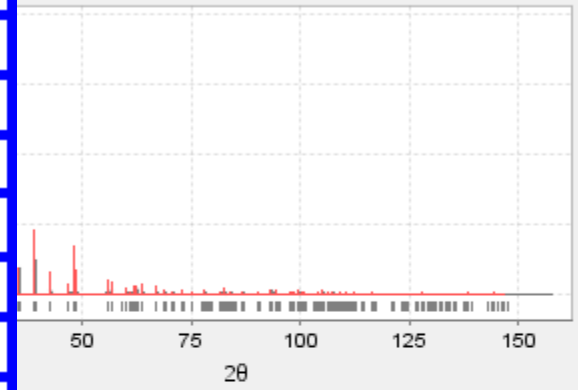
- Fixed Slit Intensity
- Variable Slit Intensity
- Integrated Intensity

Diffraction Patterns:

- Simulated Profile
- Raw Diffraction Data (PD3)

2θ	d(Å)	I	h	k	l
22.8762	3.884230	54	0	1	2
29.4493	3.030520	999	1	0	4
31.9691	2.797170	122	0	0	6
35.4526	2.529900	89	1	1	0
39.0425	2.305150	229	1	1	3
42.6132	2.119890	80	2	0	2
46.7341	1.942110	34	0	2	4
48.0433	1.892200	166	0	1	8
48.4764	1.876300	81	1	1	6
55.7243	1.648200	51	2	1	1
56.5962	1.624860	44	1	2	2

Fixed Slit Intensity



Fixed Slit Intensity — 01-077-6301 (Calculated)

PDF #: 01-077-6301 Status: Altern

Pressure/Temperature: Ambient

Chemical Formula: Na (N O3)

Structural Formula:

Empirical Formula: N Na O3

Weight %: N16.48 Na27.05 O56.47

Atomic %: N20.00 Na20.00 O60.00

ANX: ABX3

Compound Name: Sodium Nitrate

Mineral Name:

Common Name:

d(Å)	Int
3.88	10
3.04	100
2.797	20
2.536	10
2.309	20
2.122	15
1.945	5
1.895	20
1.881	10
1.650	10
1.629	5

History

File Help

Open... Ctrl+O

Save... Ctrl+S 1

Print... Ctrl+P

Close

	Description	Hits
		40,774
Search #3	{Strong Line = 1.895(.08)Å}	39,152
Search #4	{Long Line = 3.88(.08)Å}	33,756
Search #1	{Strong Line = 3.04(.08)Å} And {Strong Line = 2.309(.08)Å} And {Strong Line = 1.895(.08)Å} And	56

Results

Rename...

Delete

Delete All

Combined Searches (56)

Description	Operation
{Strong Line = 3.04(.08)Å}	<input checked="" type="radio"/> And <input type="radio"/> Or
{Strong Line = 2.309(.08)Å}	
{Strong Line = 1.895(.08)Å}	
{Long Line = 3.88(.08)Å}	

Combined Results

Add to Past Searches

Delete

Using the History Window, click on File >> Save...(1). This will bring up the “Save” Dialog Box. Then give the file a name, in this case, call it “NaNO3_verification” (2), and click the “Save” button (3).

You terminate the program, go home and come back the next day. You wish to retrieve your work.

Save

Save in: history

Recent Items

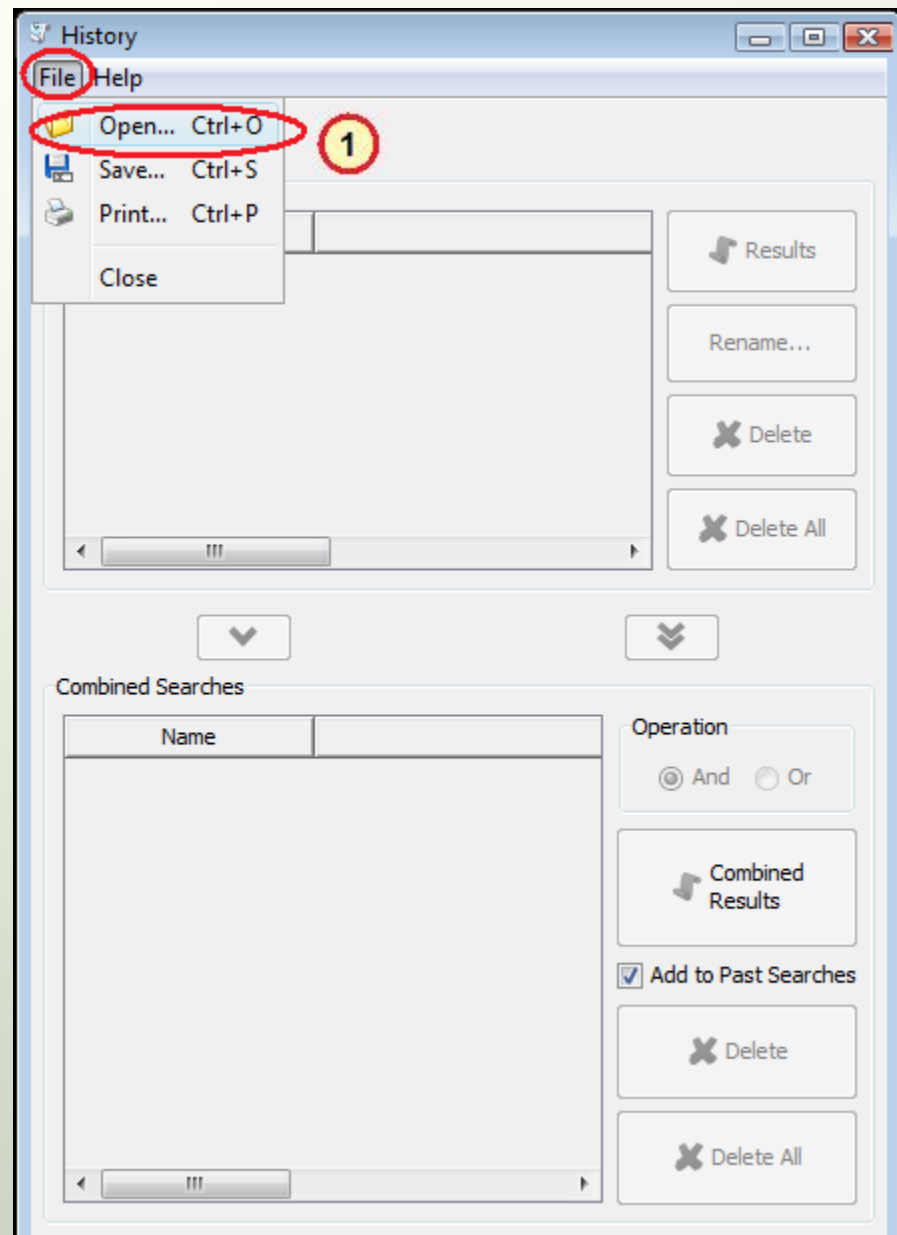
Desktop

File name: NaNO3_verification.xml 2

Files of type: ICDD XML (*.xml)

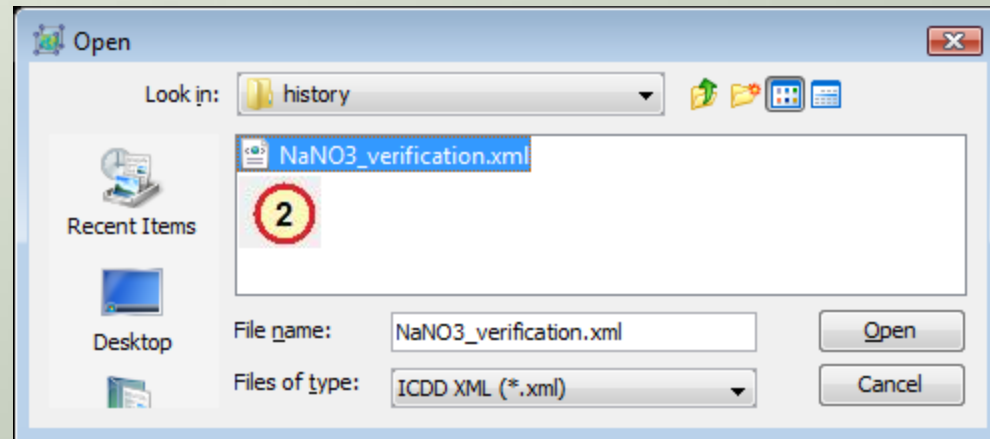
Save 3

Cancel



Go to Tools >> History and bring up the History Window.

Go to File >> Open...(1) and launch the "Open" Dialog .
Select the File "NaNO3_verification.xml" (2).



The Search comes up in the “Past Searches” list. You select “Search #5” and click On the “Results” Button, and your original Search is restored.

PDF-4+ 2011
File Edit Tools Window Help

History

Past Searches

Name	
Search #4	{Long Line = 3.88(.08)Å}
Search #5	{Strong Line = 3.04(.08)Å} And {Long Line = 3.88(.08)Å}

Results

Rename...

Delete

Delete All

Combined Searches

Name	Operation
	<input checked="" type="radio"/> And <input type="radio"/> Or Combined Results <input checked="" type="checkbox"/> Add to Past Searches Delete Delete All

Results - {Strong Line = 3.04(.08)Å}...

File Edit Fields Results Indexing Help

Results (56 of 316,291)

Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name
01-077-6301	S	Na (N O3)	Sodium Nitrate
01-078-3262	I	Ca (C O3)	Calcium Carbonate
01-078-4614	S	Ca (C O3)	Calcium Carbonate
01-079-2056	S	Na N O3	Sodium Nitrate
01-083-1762	B	Ca (C O3)	Calcium Carbonate
01-085-0849	I	Ca (C O3)	Calcium Carbonate
01-085-0850	I	Na (N O3)	Sodium Nitrate
01-085-1464	B	Na (N O3)	Sodium Nitrate
01-086-2334	S	Ca (C O3)	Calcium Carbonate
01-086-2336	S	(Mg.129 Ca.871) (C O3)	Magnesium Calcium Carbonate
01-089-2828	I	Na (N O3)	Sodium Nitrate
04-001-7249	P	Ca (C O3)	Calcium Carbonate

Search Description

{Strong Line = 3.04(.08)Å} And {Strong Line = 2.309(.08)Å} And {Strong Line = 1.895(.08)Å} And {Long Line = 3.88(.08)Å}

Calculations

Mean: Median: ESD:

Conclusion

By Combining Results with the History Window, you can perform more sophisticated searches while assessing their performance and accuracy.

By Saving Combined Results, you can share your work with colleagues and provide documentation more easily.



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

International Centre for Diffraction Data

12 Campus Boulevard

Newtown Square, PA 19073

Phone: 610.325.9814

Toll Free Number in US & Canada: 866.378.0331

Fax: 610.325.9823