

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 20 per minute and read rough 20's and I's.

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

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

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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



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

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File Edit Tools Window Help



PDF-4+ 2012

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 59,839 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.

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earch #3	{Strong Line = 1.895(.08)Å} And {Not Status (Deleted)}	39,660	3 🗶 Delete
earch #4	{Long Line = 3.88(.08)Å} And {Not Status (Deleted)}	33,796	Delete All
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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. However, you will be able to retrieve the top list after you save it.

Now click Button 6.



File Edit Tools Window Help

PDF-4+ 2012

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).

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🗟 Na (N O3) - 01-077-6301		Sodium N	litrat	e.	But	now you wa	ant to sav	ve your search 📃 🗖 📼 🕰
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PDF Experimental Physical Crystal	Ontical Stru	icture Miscellan		2 Defer	ences	1.881	10	
PDF #: 01-077-6301	Optical Sea		Sta	atus:	Altern	1.650	10	QM: Star (S)
Pressure/Temperature: Ambient						1.629	5	
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:								



History				
ile Help Open Ct Save Ct	rl+0 rl+5 1			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
Print Ct Close	rI+P Description g Line = 2.309(.08)Å} And (Not Status (Deleted)}	Hits 40,164	Results	"NaNO3_verification" (2), and click the "Save" button (3).
Search #3	{Strong Line = 1.895(.08)Å} And {Not Status (Deleted)}	39,660	Rename	You terminate the program, go home and come back the next day. You wish to retrieve your
Search #4	{Long Line = 3.88(.08)Å} And {Not Status (Deleted)}	33,796	E X Delete	
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Search #1	{Strong Line = 3.04(.08)Å} And {Not Status (Deleted)}	59,839	And Or	File name: NaNO3_verification.xml Save Desktop Files of type: ICDD XML (*.xml) Cancel
Search #2	{Strong Line = 2.309(.08)Å} And {Not Status (Deleted)}	40,164	Combined Results	
Search #3	{Strong Line = 1.895(.08)Å} And {Not Status (Deleted)}	39,660	Add to Past Searches	
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Add to P	Past Searches				
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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.

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∛ History	Strong Line = 3.04(.08)Å}								
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Search #4	{Long Line = 5.66(.06)A} And {h	Rename	PDF #	QM	Chemical Formula	0	Compound Name		
			01-077-6301	S	Na (N O3)	Sodium Nitra	ate	3.(
Search #5 {Strong Line = 3.04(.08)Å} And { And { {Strong Line = 2.309(.08)Å} And { Image: Comparison of the second s			01-078-3262	1	Ca (C O3)	Calcium Carbonate :		3.(
			01-078-4614	S	Ca (C O3)	Calcium Carbonate		3.(
			01-079-2056	S	Na N O3	Sodium Nitrate		3.(
	01-085-0849	1	Ca (C O3)	Calcium Carbonate		3.(
			01-085-0850	1	Na (N O3)	Sodium Nitrate		3.(
	01-085-1464	В	Na (N O3)	Sodium Nitrate		3.(
Combined Searches	01-086-2334	S	Ca (C O3)	Calcium Carbonate		3.(
Name		Operation	01-086-2336	S	(Mg.129 Ca.871) (C O3)	Magnesium Calcium Carbonate		2.1	
) And Or	01-089-2828	1	Na (N O3)	Sodium Nitrate		3.(
			04-001-7249	P	Ca (C O3)	Calcium Car	rbonate	3.(
		Combined	04-002-7275	P	Na (N O3)	Sodium Nitra	ate	3.(
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Add to Past Se			Search Description Calculations						
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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