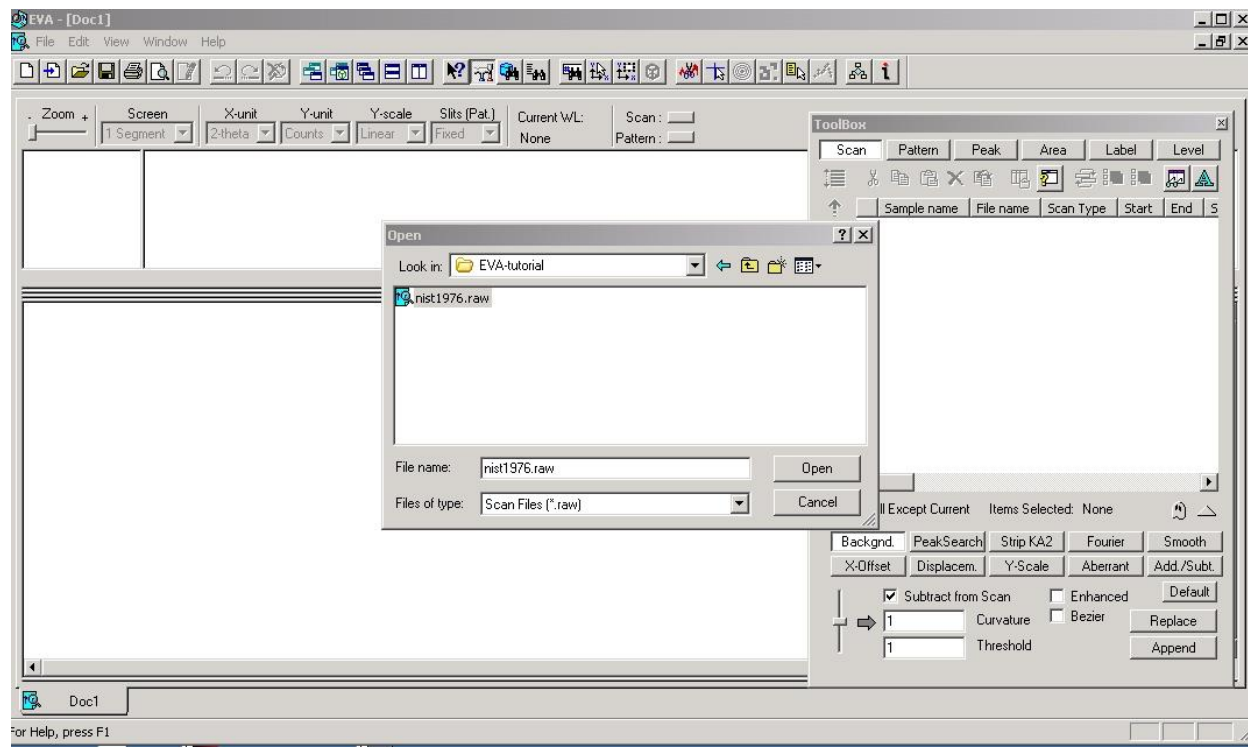



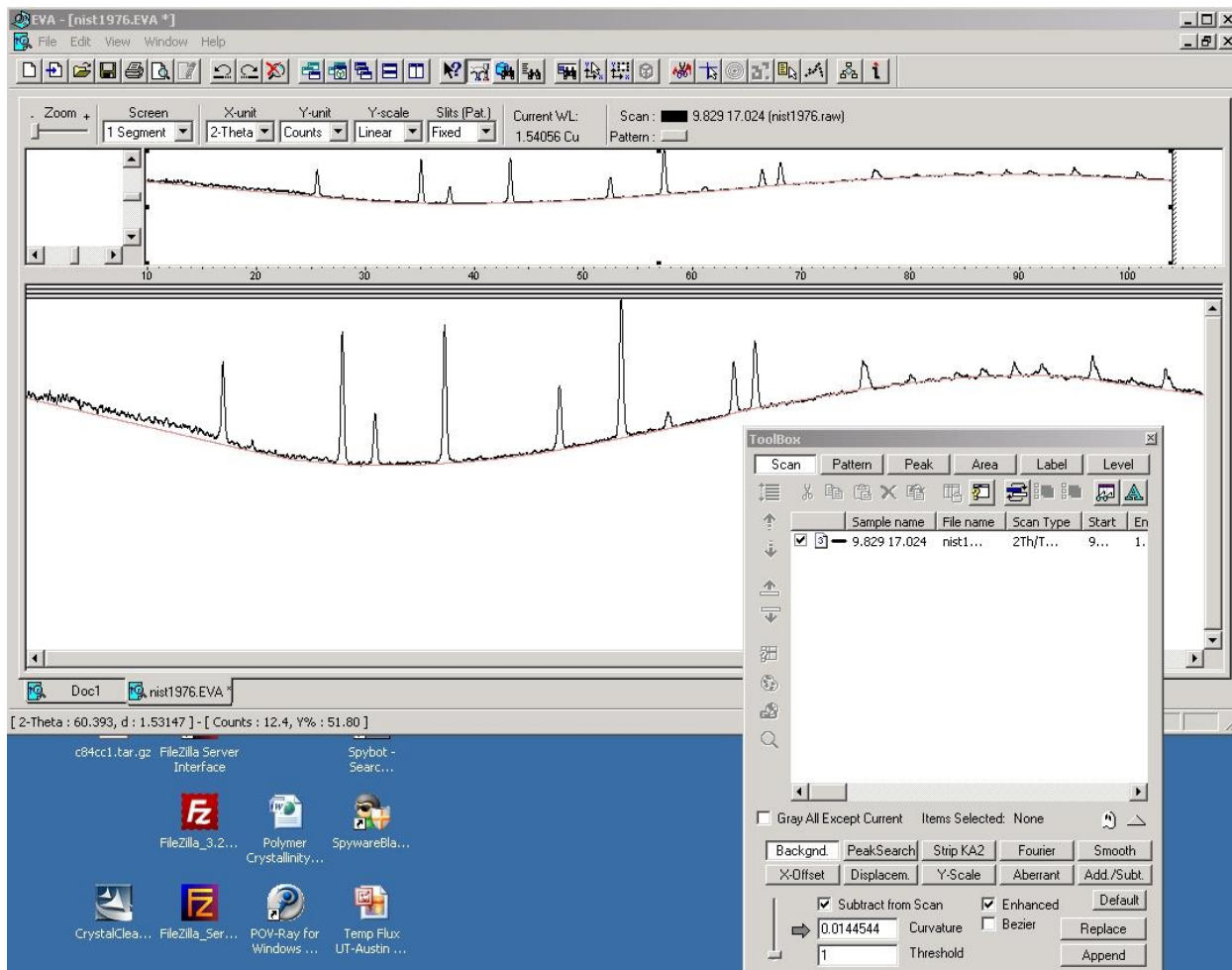
Using EVA to analyze the .raw scans



Once you have a .raw file, you can open the Bruker EVA program,



Open your .raw data file. Look at the top of the EVA gui. The various icons will enable you to perform various tasks. The most used icon will be ScanTools, , where you can manipulate the pattern, do a background correction, generate a peak list file, etc.

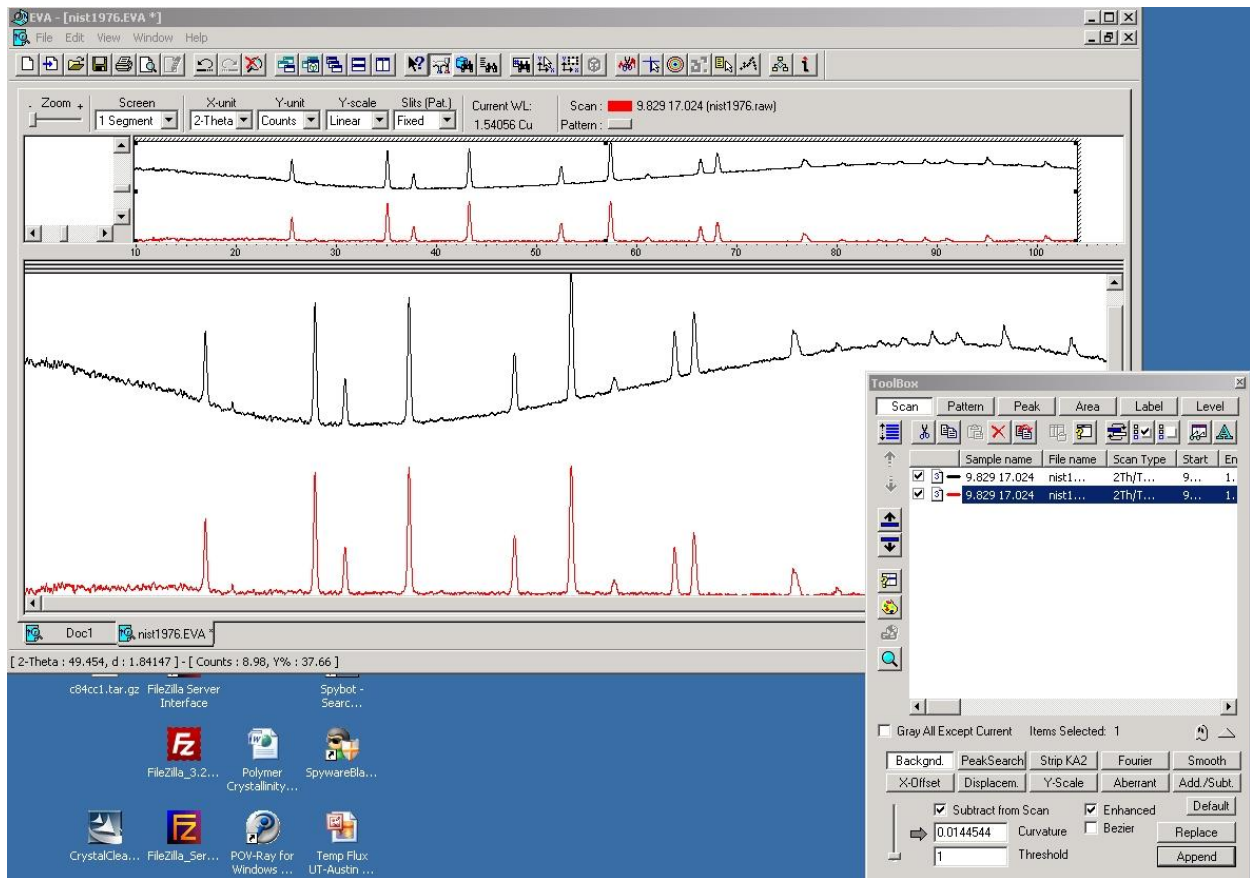


By default, you will see two windows (panes). The top pane displays the original pattern. You can use the mouse to zoom in on selected portions of the pattern to work on as displayed in the lower pane. The bottom pane is the working pane.

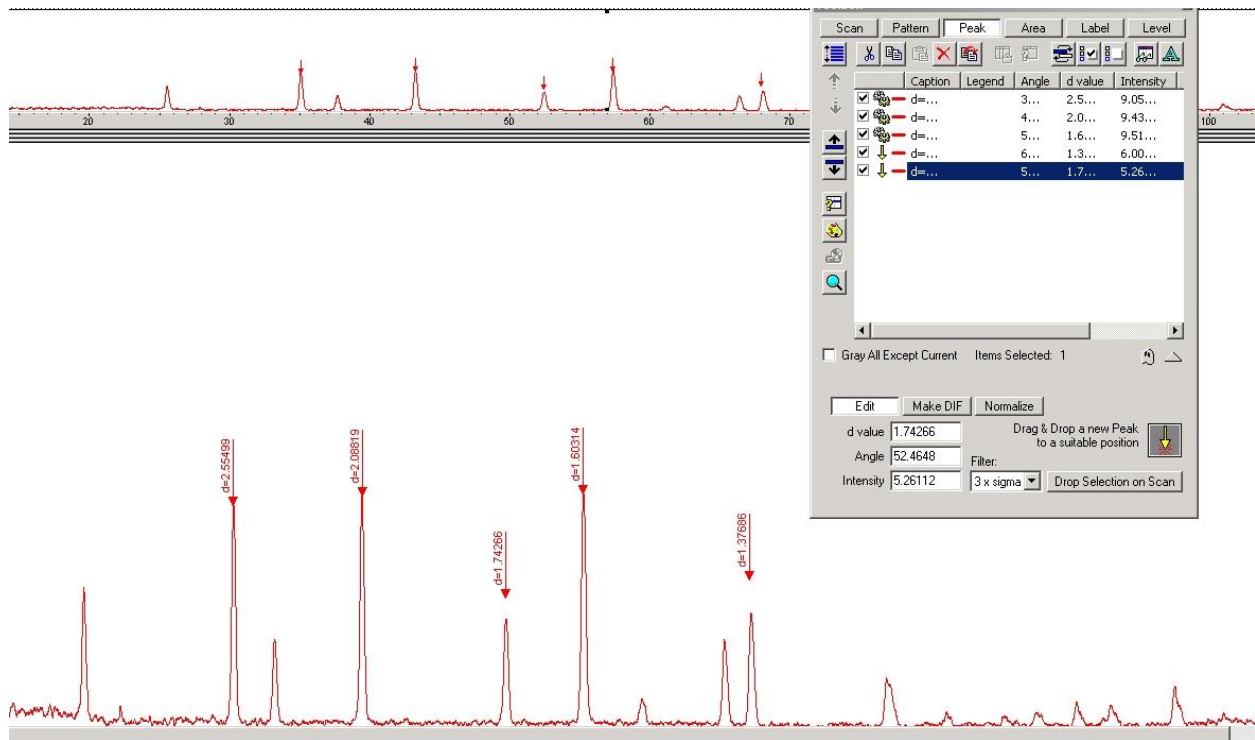
To correct for background using the Spider data, use the Enhanced form. You can adjust the correction parameters using the slide bar to the lower left of the ScanTools menu. Most of the default parameters can be adjusted in this way. Some menus have double sided arrows in blue,



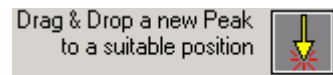
, that you can use to increase or decrease the numerical ranges listed to the left. In addition, most menus have a replace and an append button. Replace will replace the original pattern with the corrected pattern. Append will keep the original and display both patterns in the adjustment window. You will see the two patterns with different colors. The two will also be listed in the ScanTools window. By doing this, you will not change the raw data.



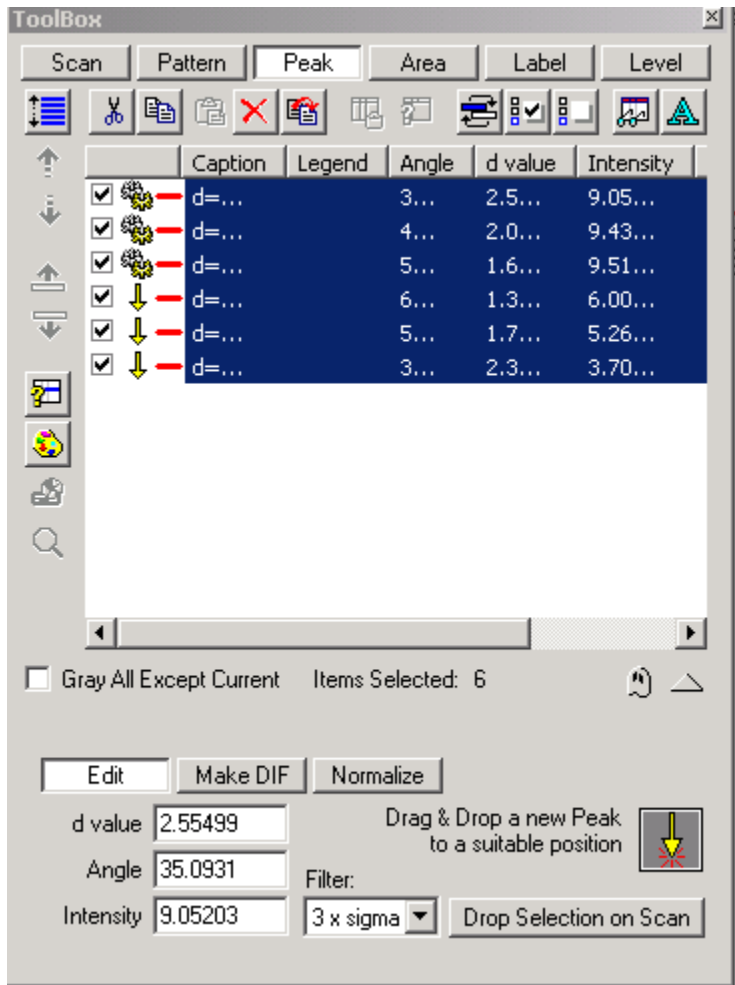
Double clicking on the black check box will remove that pattern from the display window. You can do a pattern search either on the scan file or on a list of peaks you generate from that scan. To generate a peaks list, which is called a .dif file in Brukerese, click the PeakSearch button on ScanTools. Move the slide bar on the left to select/deselect peaks. You can change the working range listed in the Slider region by clicking one of the double sided blue arrows. If you can't get all the peaks you wish to list, select Append To List.




You can add additional peaks manually using the Drag&Drop button,

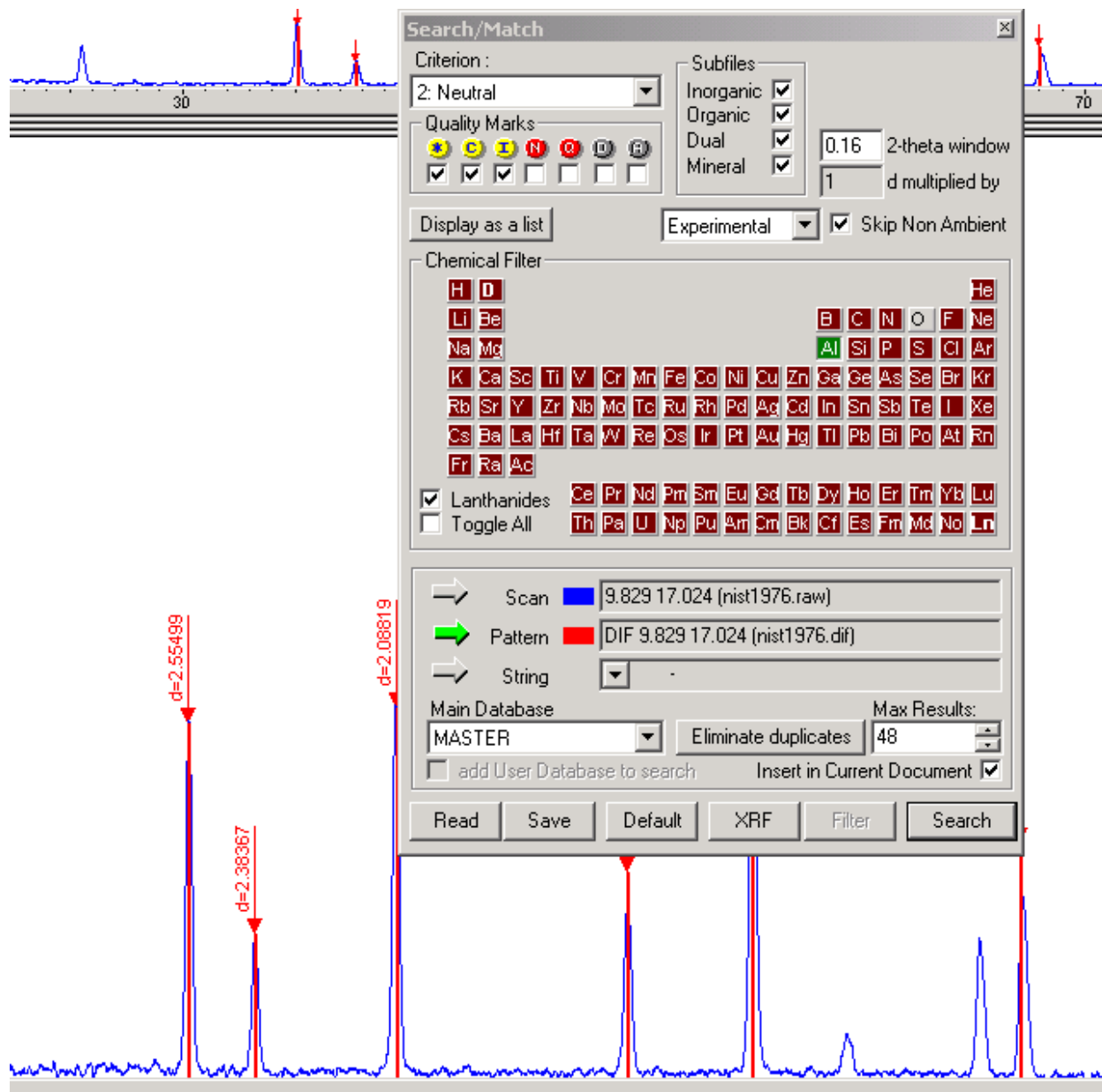


Left click on the arrow and drag the mouse pointer to one of the desired peaks and release the mouse. The newly added peak will be shown in blue in the peak list area. If you don't like where you placed the arrow, delete the peak and do it again. When you have added all the peaks you want, be sure to highlight all the peaks before hitting the MakeDif button.



A second menu will be displayed in case you need to make some changes. If you are satisfied with the result, hit MakeDif again and a DIF file will be created. Now you can search the PDF file using either the raw scan file or the peaks list file. You will be searching the same PDF file that you use in JADE.

You can run the Bruker Search/Match utility by clicking . The Search/Match menu will be displayed.



You can use the periodic table to select particular atoms that either must be in the pattern, that are possibly in the pattern or can not be in the pattern. Atoms that must be in the pattern will be green (Al above), those that can't be in the pattern are in violet and those that may or may not be in the pattern are grey (O above). You can search using the scan data, or the peak list file (Pattern) as selected above. The quality marks allow you to limit the patterns searched. Yellow refer to the 'best' available patterns, red refer to patterns that either haven't been fully vetted or are of questionable quality and grey are patterns that have been superseded by more modern patterns.

Max. results limits the number of hits displayed. The box next to Insert in Current Document should be checked to list the hits in the ScanTools menu. To the right of the Search/Match icon,



, brings up a listing of the matching entries.

Search Results

SS-VW-PPPP	Compound Name	Formula	Mtc	nM	FQM	f
00-046-1212	Corundum, syn	Al2O3	5	1	10.21	7
00-010-0173	Corundum, syn	Al2O3	6	1	17.70	2
00-050-1496	Aluminum Oxide	Al2O3	4	7	133.0	3
00-058-0334	Aluminum Oxide	Al2O3	1	5	13...	4
00-056-1186	Aluminum Oxide	Al2O3	4	6	29...	5
00-050-0741	Aluminum Oxide	Al2O3	1	6	30...	6
00-026-0031	Aluminum Oxide	Al2O3	1	4	51...	7
00-023-1009	Aluminum Oxide	Al2O3	2	7	61...	8
00-035-0121	Aluminum Oxide	Al2O3	1	8	90...	9
00-046-1215	Aluminum Oxide	Al2O3	1	13	62...	10

Drag & Drop the selection in a window

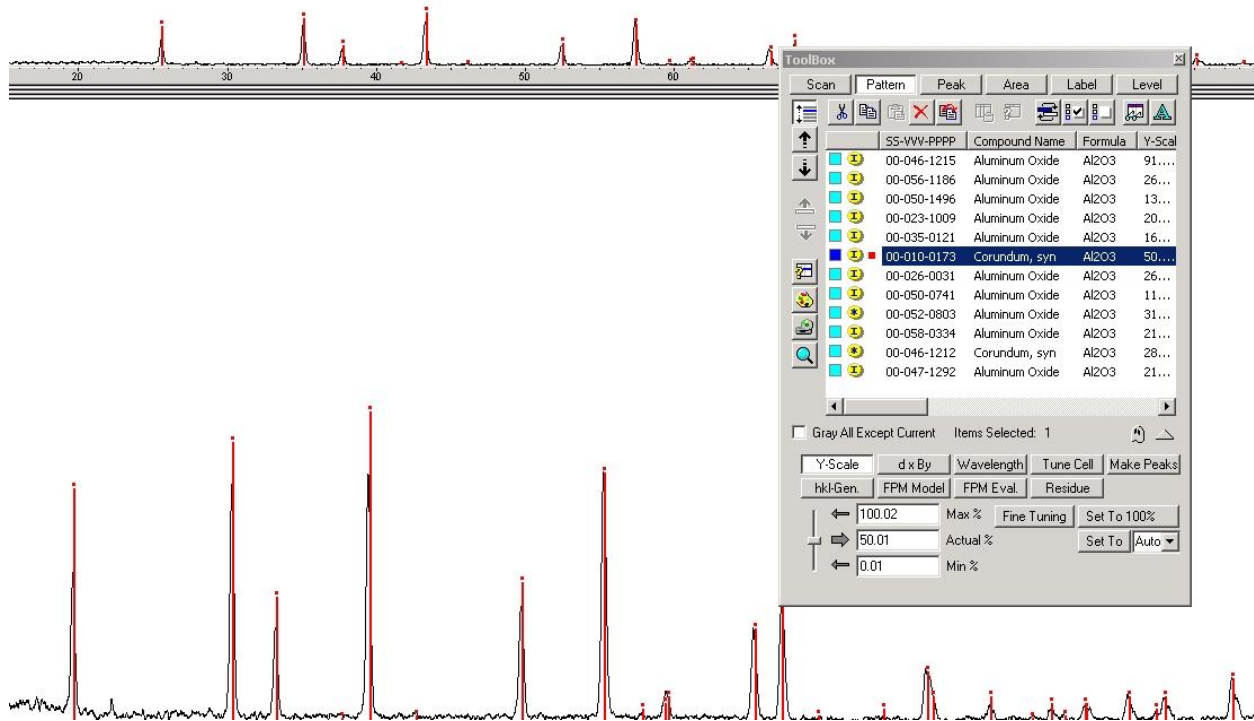
Statistics

Search On : Pattern: DIF 9.829 17.024 (nist1976.dif)
d multiplied by : 1.
2-theta offset :
Displacement :
2-theta window : 0.160
Criterion : 2: Neutral
Database : C:\DPRD\PDF2008.4CA
Total number : 211107
Match Chem./Subfile : 13
Matching Intensity : 10
Elapsed Time : 2.9

Read Save Delete Selection Reset List

The number of patterns with matching chemistry and peaks is listed here. For this sample, I have 10 total matches. I asked that 48 be listed so I got all the matching entries. Had the number of matches exceeded 48, there is a chance that I would have missed an important match.

The search results will appear in the ScanTools window.



There is limited space in the ScanTools window. You can use the slide bar to move through the listing. You can expand each entry in the list by expanding the space allowed for each entry.

Length	System	a	b	c	alpha	beta
Ort...		7.93400	7.95600	1... 9...		9...
Tet...		7.96310	7.96310	2... 9...		9...




To see more detail concerning any matching entry, click on the CD-Rom icon on the side,

To retain that entry and continue through the list, place a check mark by the blue box,

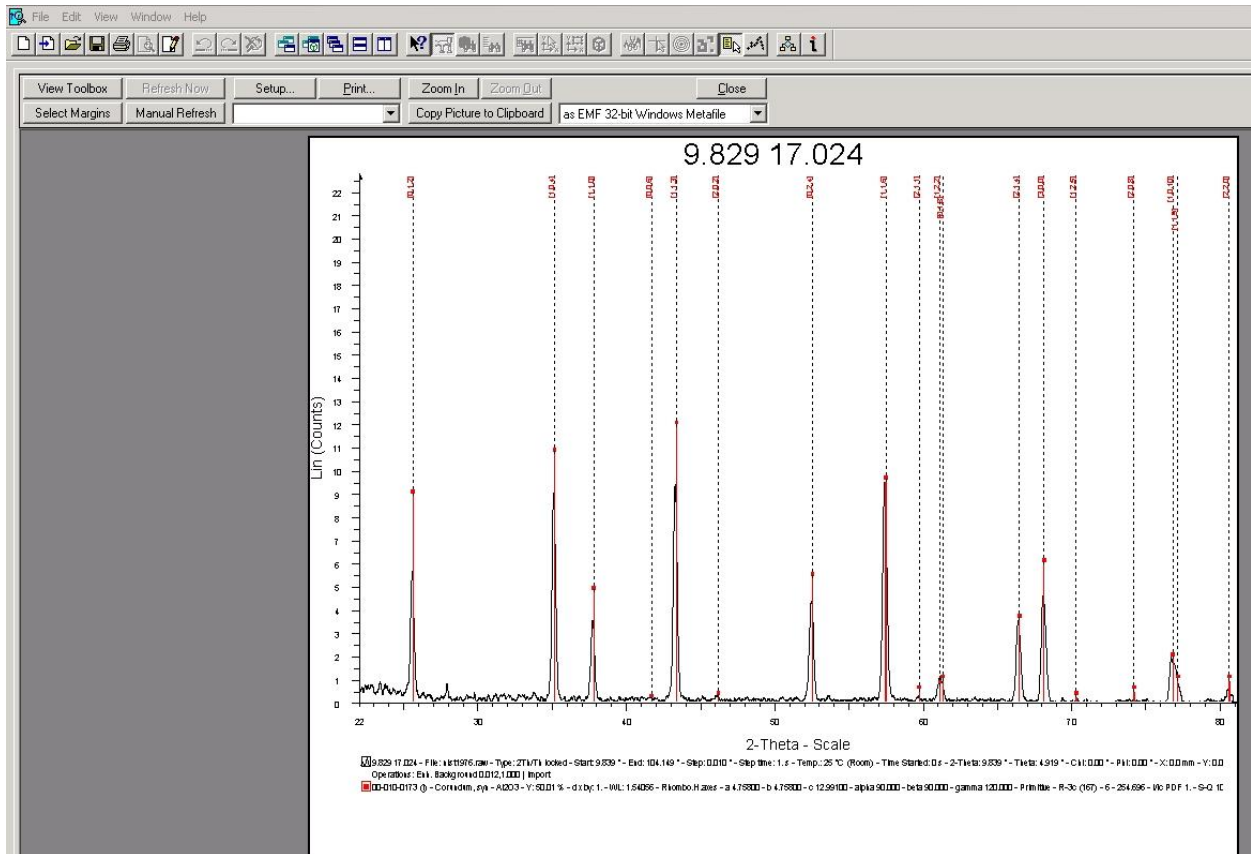
<input type="checkbox"/>		00-035-0121	Aluminum Oxide	Al2O3	16...
<input checked="" type="checkbox"/>		00-010-0173	Corundum, syn	Al2O3	50...
<input type="checkbox"/>		00-026-0031	Aluminum Oxide	Al2O3	26...



and proceed using the arrows. You can change the color of any selected entry by clicking the color palate and selecting the appropriate color.

To list the indices of each peak, the popup information menu  must be depressed AND a check mark must be in place by the selected entry. To see the hkl value, place the mouse pointer on the peak.

A nice feature of EVA is PrintPreview, which can be accessed under the File drop down menu.



The pattern can now be copied to the clipboard and inserted in MS-Office programs like Word, EXCEL and PowerPoint. There is some flexibility in the appearance of the figure using the View Toolbox menu. You can toggle the reflection indices on and off by use of the Popup menu

icon, .