

# Introduction to EVA

## A Complete Orientation to Features and Functions

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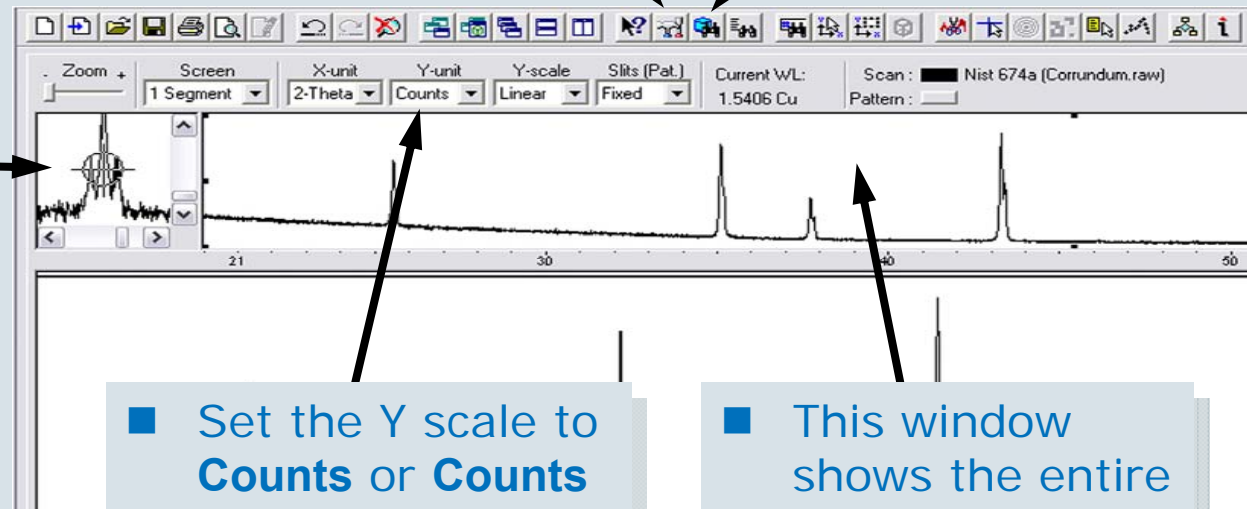
# Introduction

- EVA (short for Evaluation) is a program designed to provide the customer a quick and easy way to process data
- Primary functions include
  - Determining peak locations and FWHM
  - Comparing scans against a database (Db) of known compounds and determining the phases which are present
  - Making a scan with respect to a known standard, typically the ICDD Db file, to determine the lattice parameters and phase composition

# Layout of EVA (upper portion)

■ Toolbox      ■ Search/ Match

■ Magnified view  
of the cursor  
location



■ Set the Y scale to  
**Counts** or **Counts  
per Second**

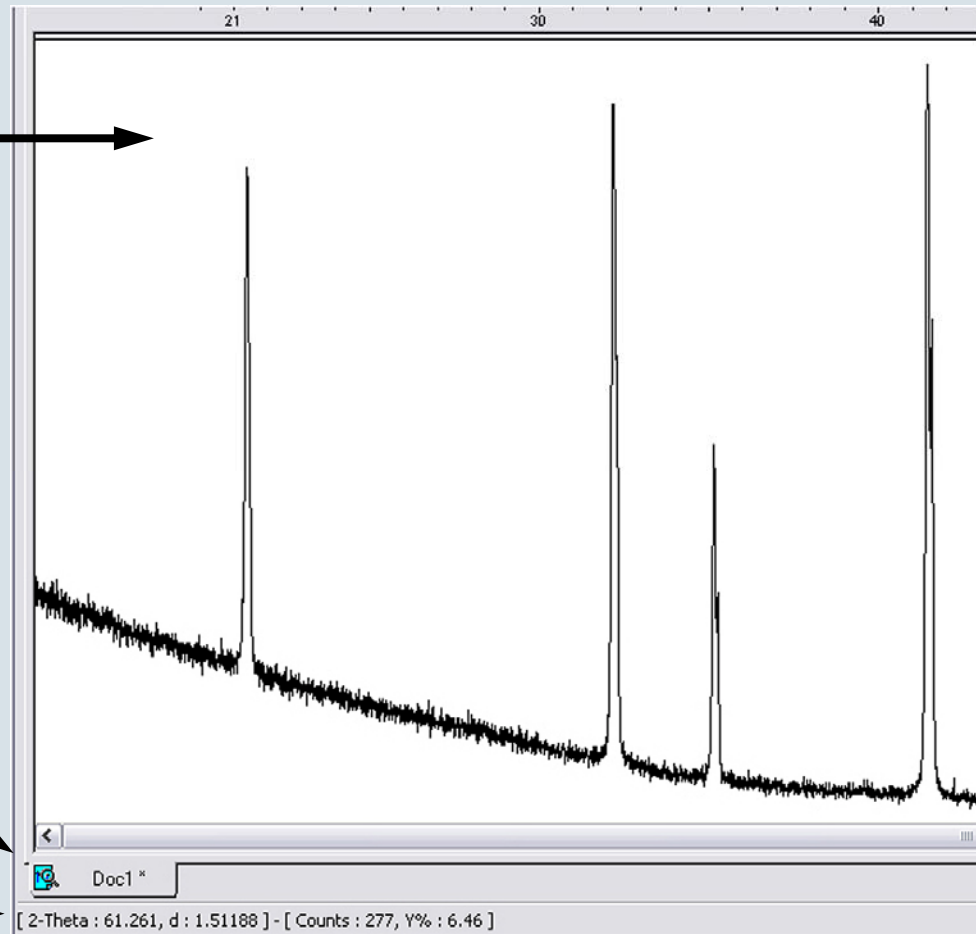
■ This window  
shows the entire  
scan

# Layout of EVA (lower portion)

- Main editing window

- Worksheet tabs

- Position of the cursor  
(coordinates)



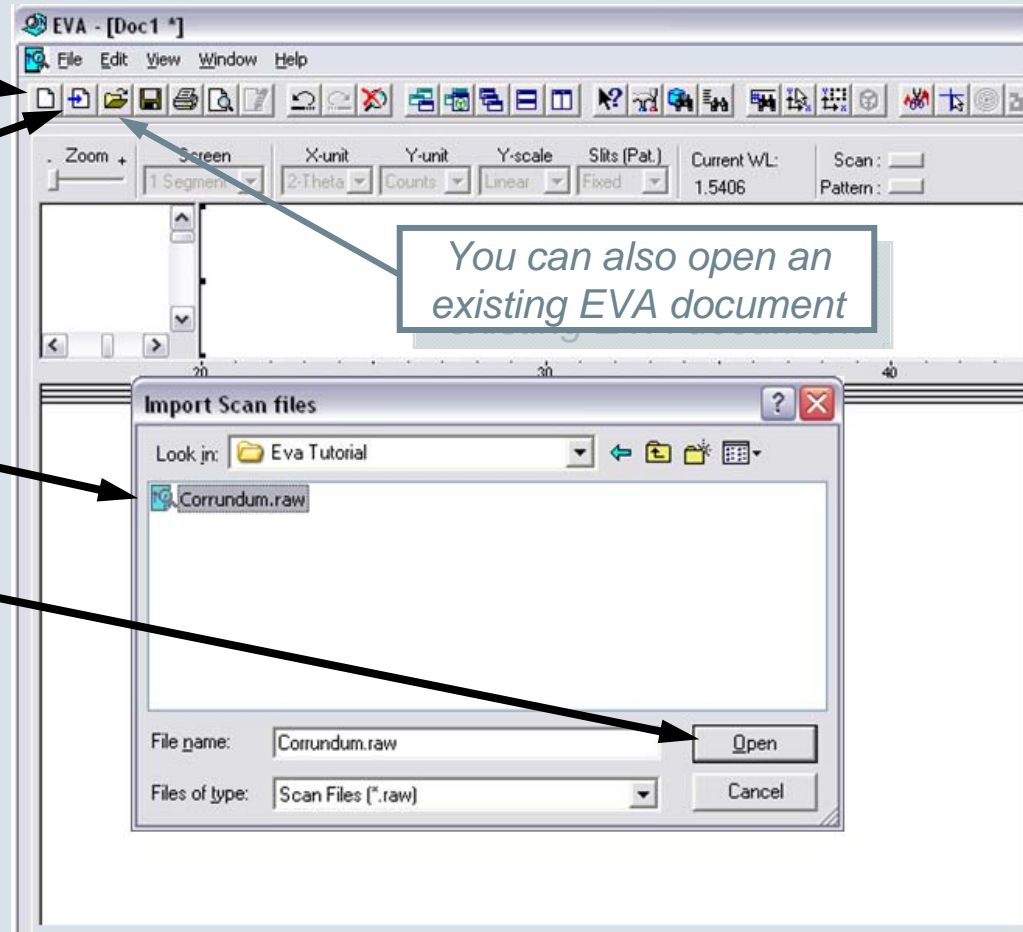
# Importing a Scan

1. Select **New Worksheet**

2. Select **Import a scan**  
(.raw file) button

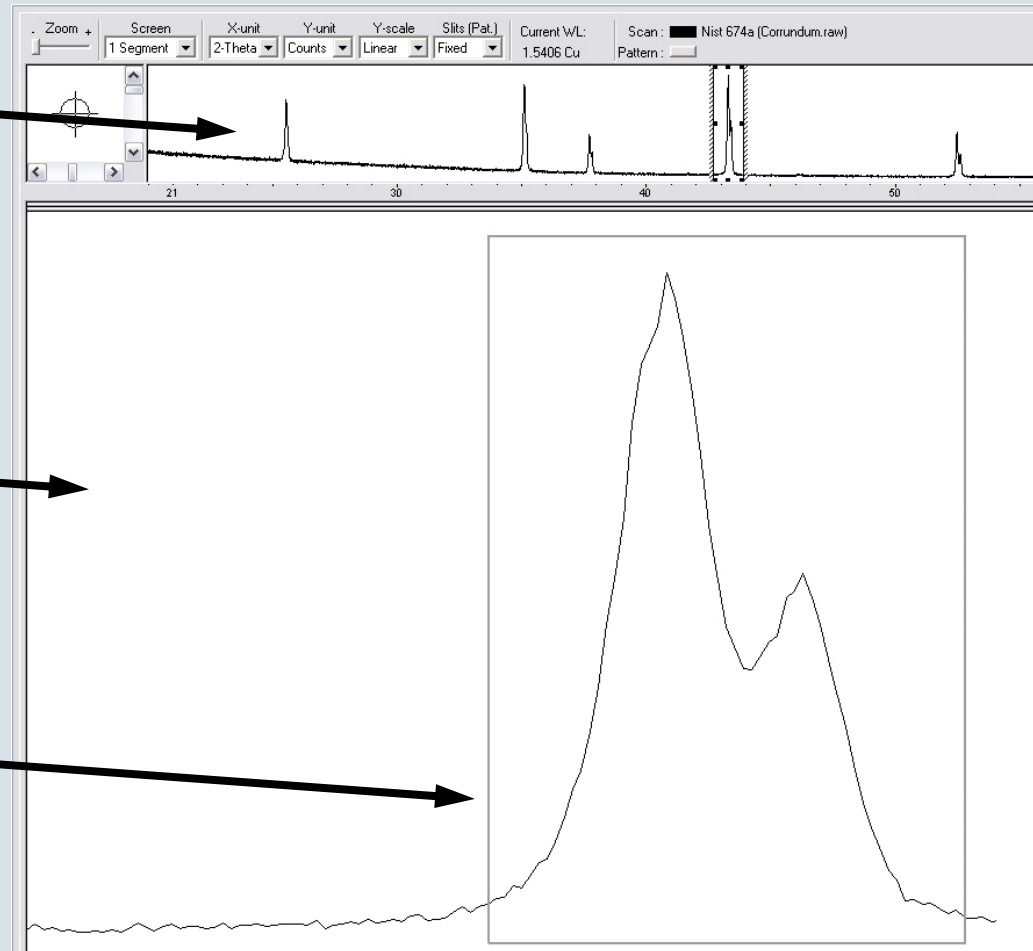
3. Select a scan with a  
mouse-click. To import  
multiple scans, press the  
[Ctrl] key while clicking

4. Select **Open**



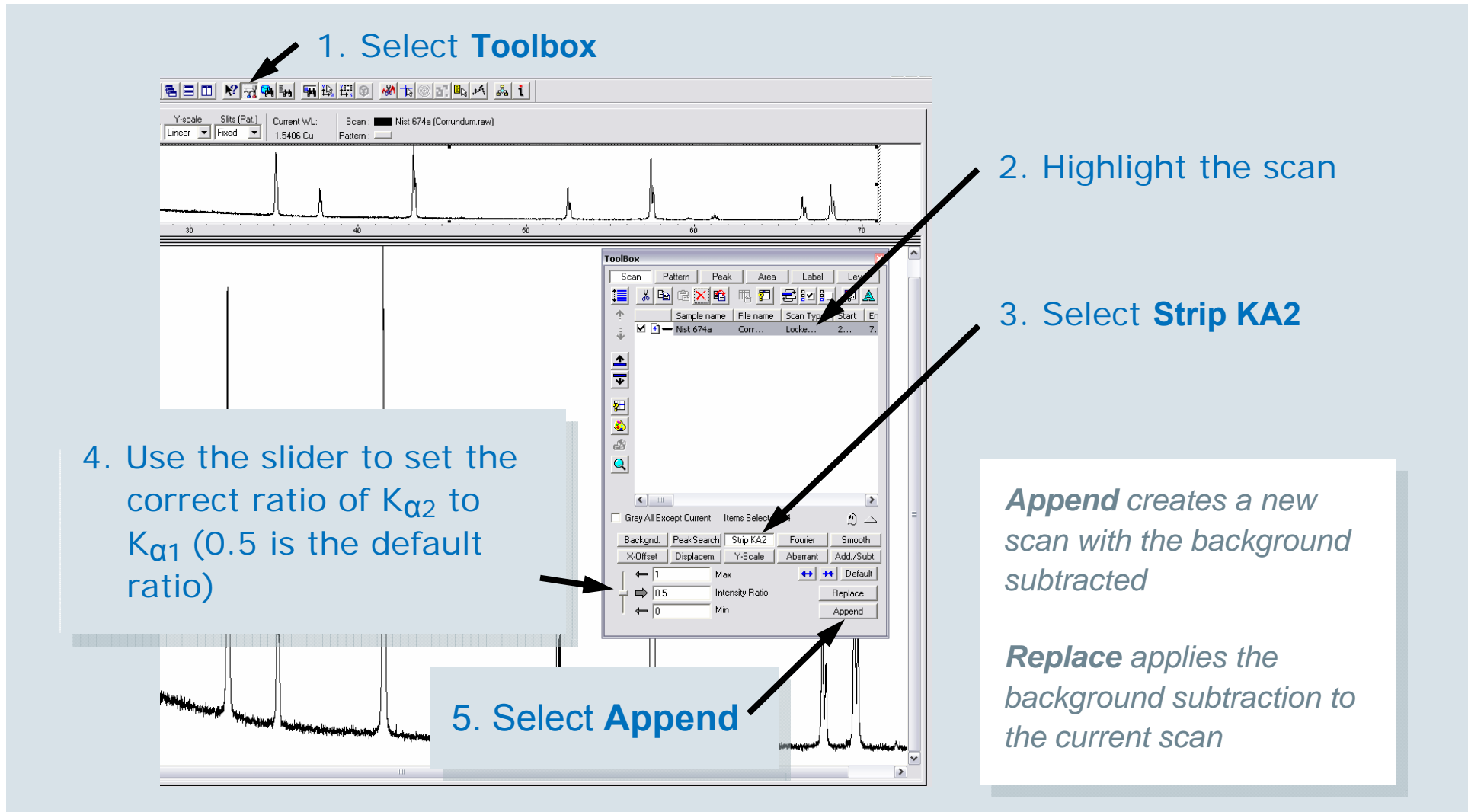
# Zooming on a Scan Range

- To un-zoom, double click in this window
- To adjust the maximum intensity for the zoomed range, double click in this window
- To zoom-in on a peak, use the mouse to draw a box over the area of interest



# Stripping $K_{\alpha 2}$

(Applicable to machines that do not have a monochromator)



1. Select **Toolbox**

2. Highlight the scan

3. Select **Strip KA2**

4. Use the slider to set the correct ratio of  $K_{\alpha 2}$  to  $K_{\alpha 1}$  (0.5 is the default ratio)

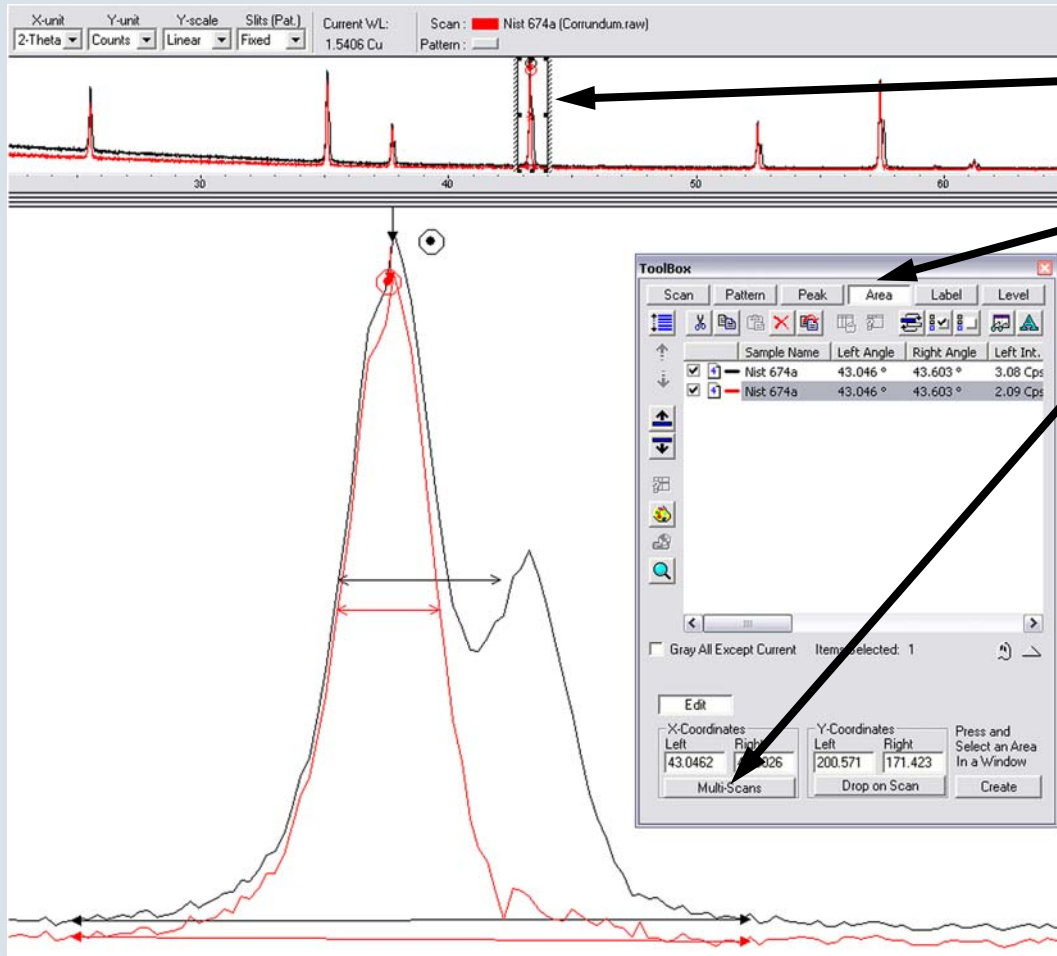
5. Select **Append**

*Append creates a new scan with the background subtracted*

*Replace applies the background subtraction to the current scan*



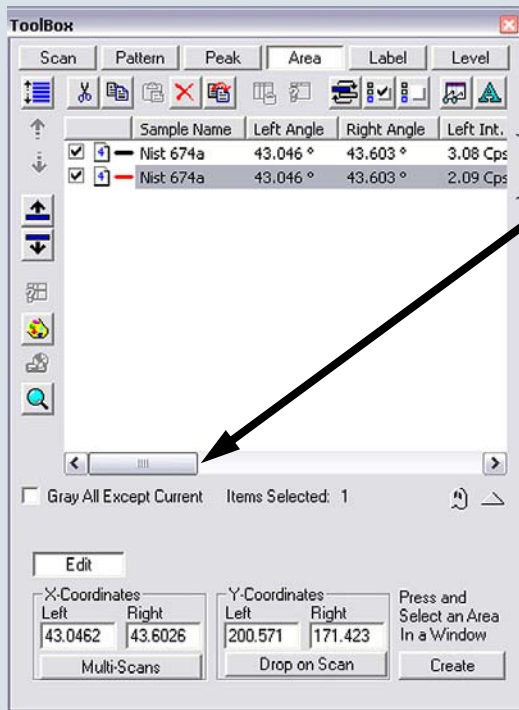
# Determining the FWHM and Position of Peaks Using the Area Function



1. Zoom in on a peak
2. Select the **Area** tab in the **Toolbox**
3. Select **Multi-Scans**
4. Select **Create**
5. Using the mouse, drag a region over the peak

*If you are interested in a single scan, highlight the scan of interest in the **Scan** tab, then select **Area**, and then select **Create***

# Determining the FWHM and Position of Peaks Using the Area Function (continued)



6. Lines have been added to the window

7. Use the scrollbar to scroll to the right to view these additional fields:

*FWHM - Full Width of the peak at Half Maximum ↔*

*Observed Maximum - Point with maximum intensity ↓*

*Chord Middle - Middle of the cord used to determine the FWHM*

*Gravity Center - Weights the determination of the peak center using the intensity ⊕*

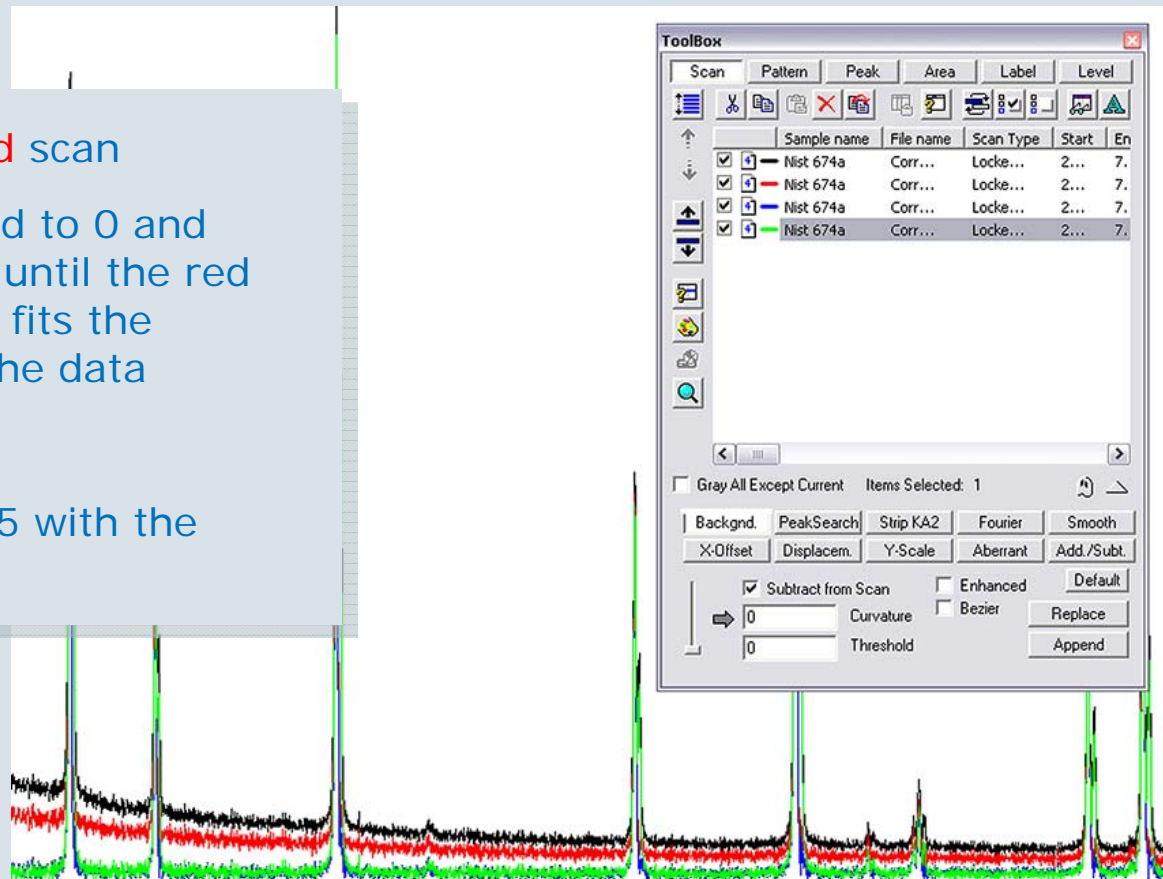
*Net Area – The area under the peak with background subtraction taken into account. Used for IQOQ*

Note that **Gravity Center**, **Chord Mid** and **FWHM** are only valid for isolated peaks!

# Subtracting the Background

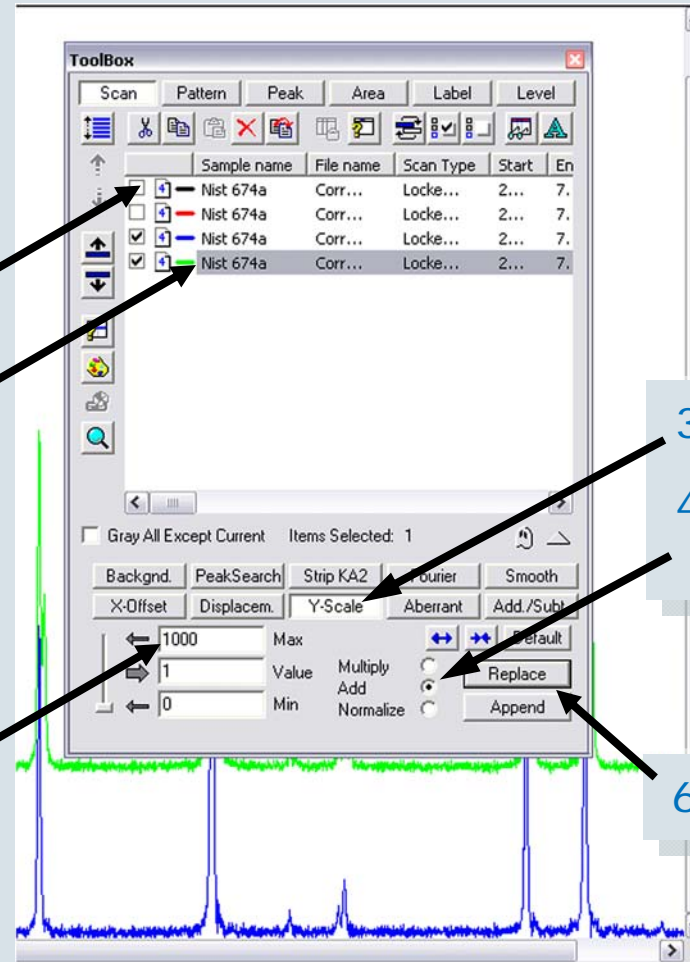
In preparation for doing a Search / Match

1. Highlight the **red** scan
2. Set the threshold to 0 and move the slider until the red background line fits the background of the data
3. Select **Append**
4. Repeat steps 1-5 with the black scan



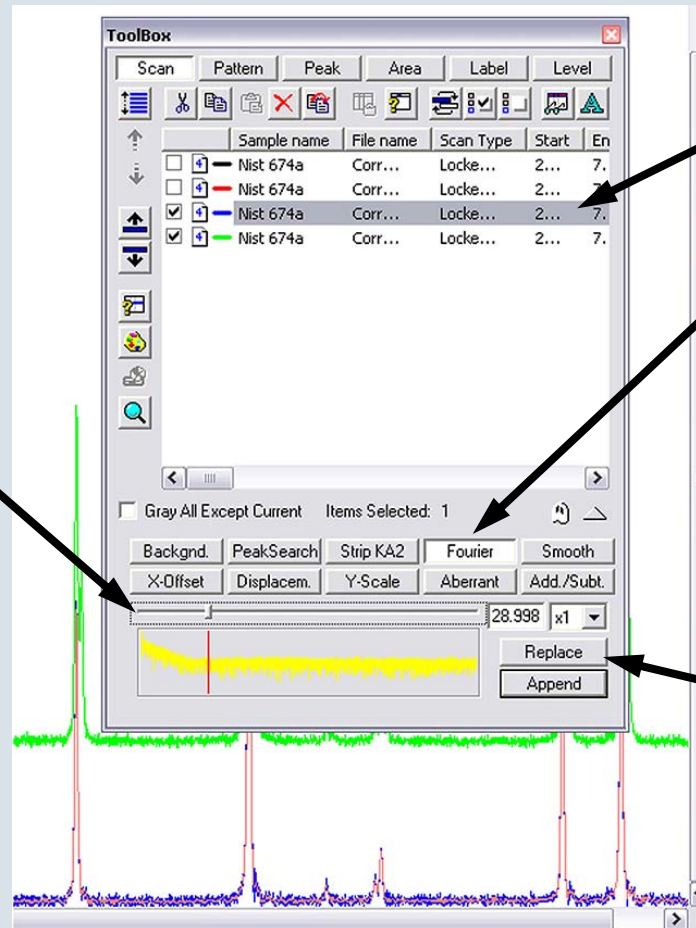
# Cleaning Up the Worksheet

1. Hide the "non background subtracted" scans by double clicking the checkbox
2. Highlight the pre-K $\alpha_2$  stripping scan
3. Select **Y-Scale**
4. Check the **Add** circle
5. Set **Max** to  $\frac{1}{4}$  the intensity of the highest peak and **Min** to 0. Then using the slide translate the scan vertically
6. Select **Replace**



# Smoothing the Scan

If the scan has an unacceptable amount of noise



1. Highlight the Scan with  $K_{\alpha 2}$  subtracted

2. Select **Fourier**  
(You could also try **Smooth** but we have gotten better results with **Fourier**)

3. Use the slider to set the red line on the right side of the bend

4. Select **Replace**

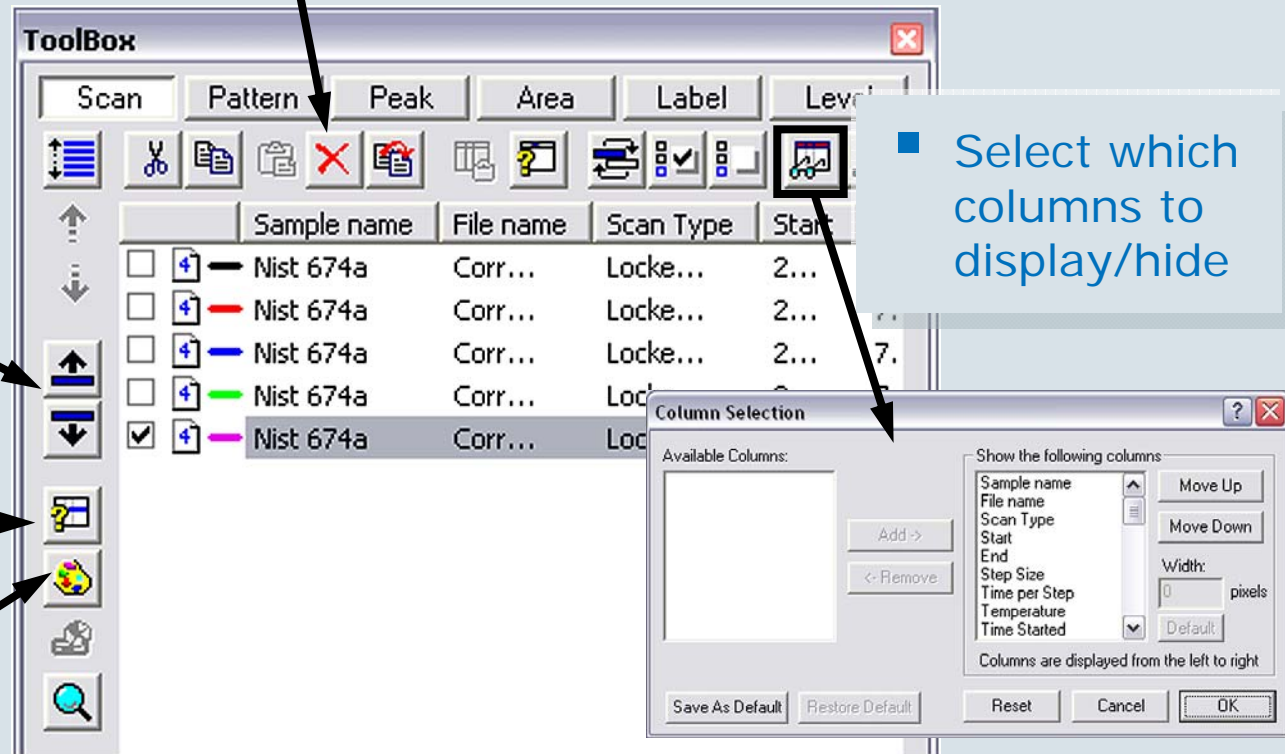
# Additional Toolbox Functions

- Delete the highlighted scan

- Move the scan up or down in the list

- Various properties of the scan

- Change the color of the scan



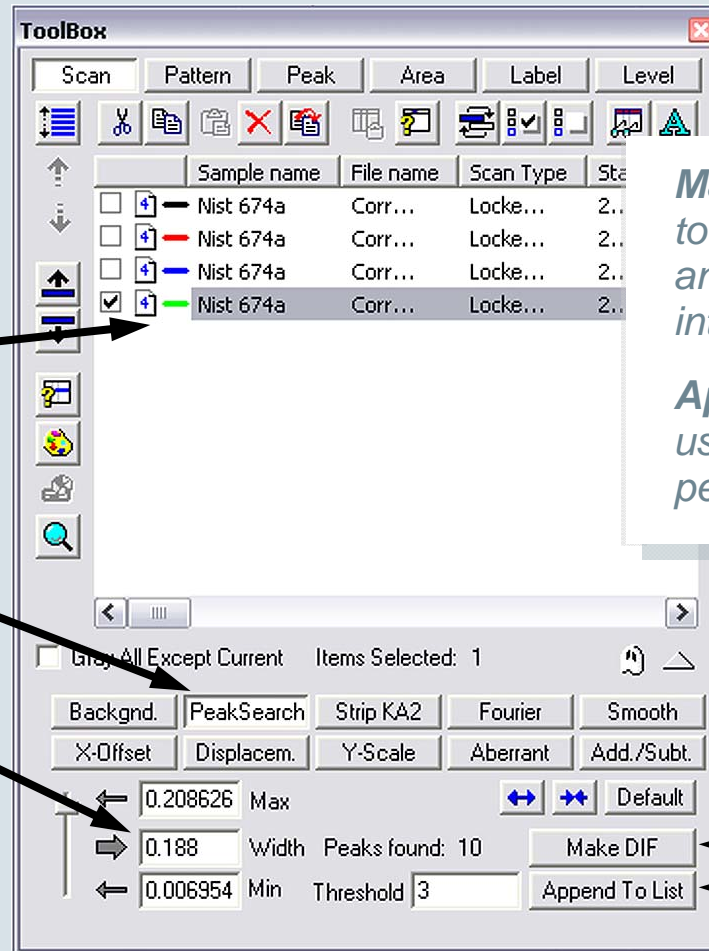
The screenshot shows the 'ToolBox' window with tabs for Scan, Pattern, Peak, Area, Label, and Level. The 'Scan' tab is active, displaying a table of scan data. A red 'X' icon in the toolbar is highlighted with a black box and an arrow pointing to the text 'Delete the highlighted scan'. A callout box on the right says 'Select which columns to display/hide' with an arrow pointing to the 'Column Selection' dialog box. The dialog box shows a list of available columns and a list of columns to be displayed. The 'Scan' tab table has the following data:

	Sample name	File name	Scan Type	Start
<input type="checkbox"/>	Nist 674a	Corr...	Locke...	2...
<input type="checkbox"/>	Nist 674a	Corr...	Locke...	2...
<input type="checkbox"/>	Nist 674a	Corr...	Locke...	2...
<input type="checkbox"/>	Nist 674a	Corr...	Locke...	2...
<input checked="" type="checkbox"/>	Nist 674a	Corr...	Locke...	2...



# Peak Search

1. Ensure that the background subtracted  $K_{\alpha 2}$  stripped scan is highlighted
2. Select **Peak Search**
3. Adjust the **Threshold** and **Width** until the peak locations are satisfactory



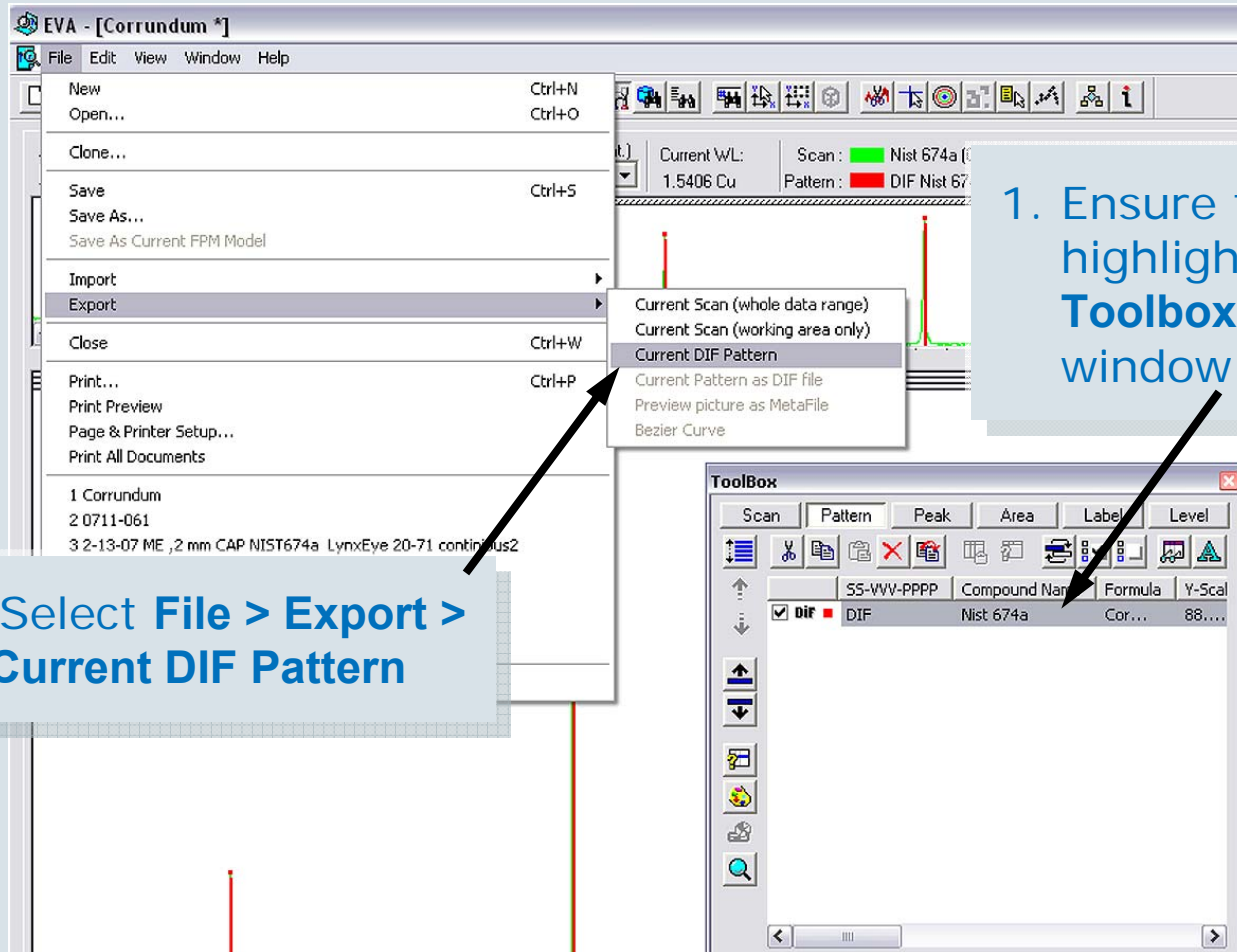
*Make a DIF is used to create a list of angles and intensities*

*Append to List is used to label the peaks in a scan*

4. Select **Make DIF** or **Append to List**

# Peak Search - Exporting the DIF

(Used to create custom patterns in a PDF Db)



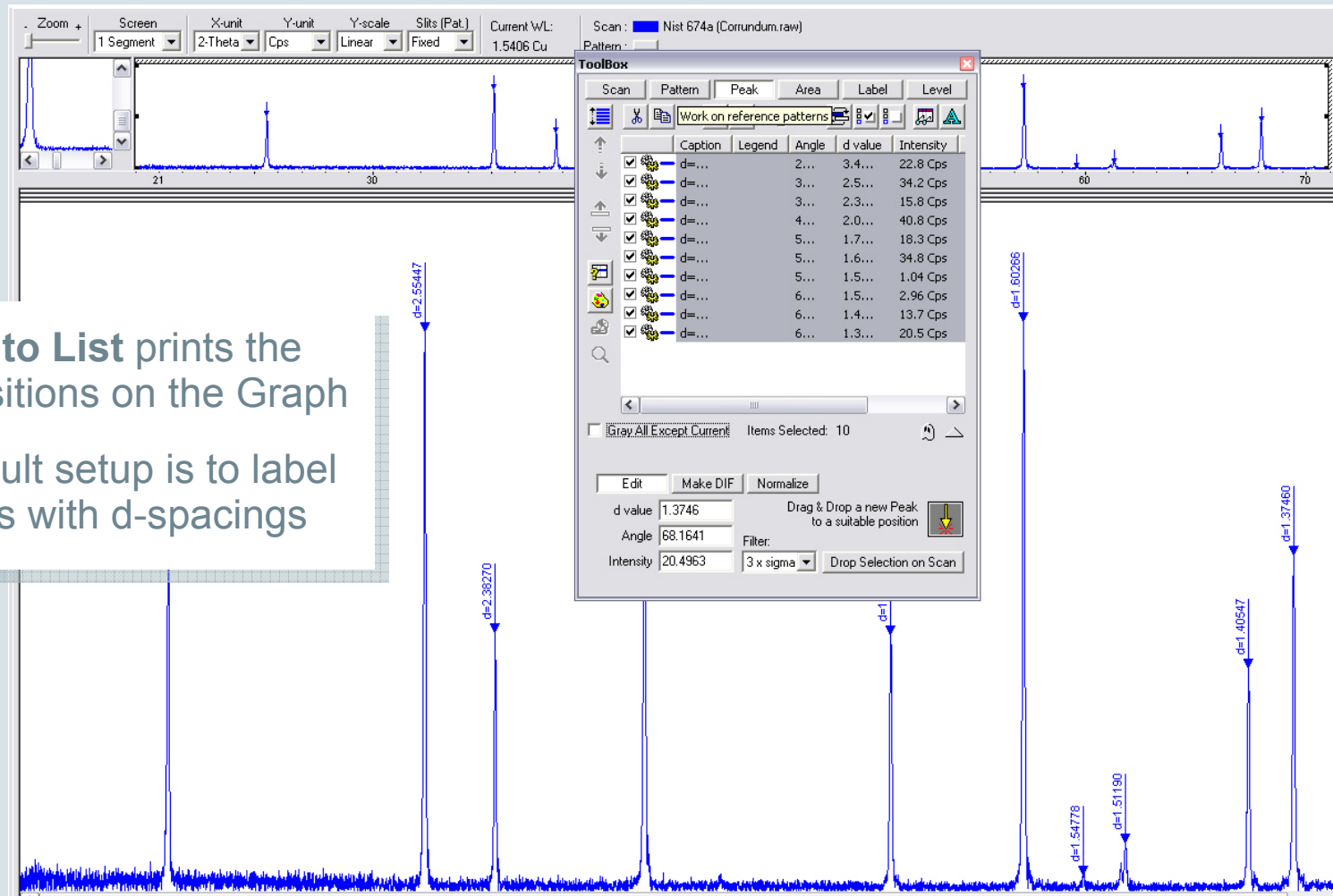
1. Ensure the DIF is highlighted in the **Toolbox: Pattern** window

2. Select **File > Export > Current DIF Pattern**

Scan	Pattern	Peak	Area	Label	Level
<input checked="" type="checkbox"/>	DIF	Nist 674a	Cor...	88...	

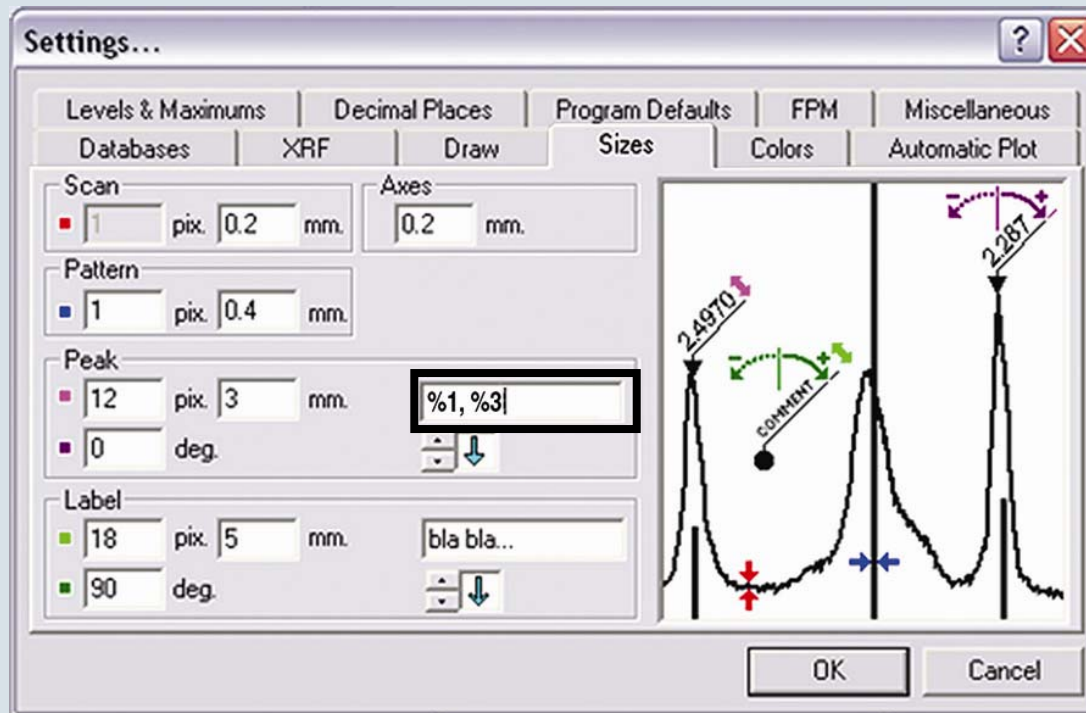


# Peak Search - Append to List



# Changing the Default Peak Label

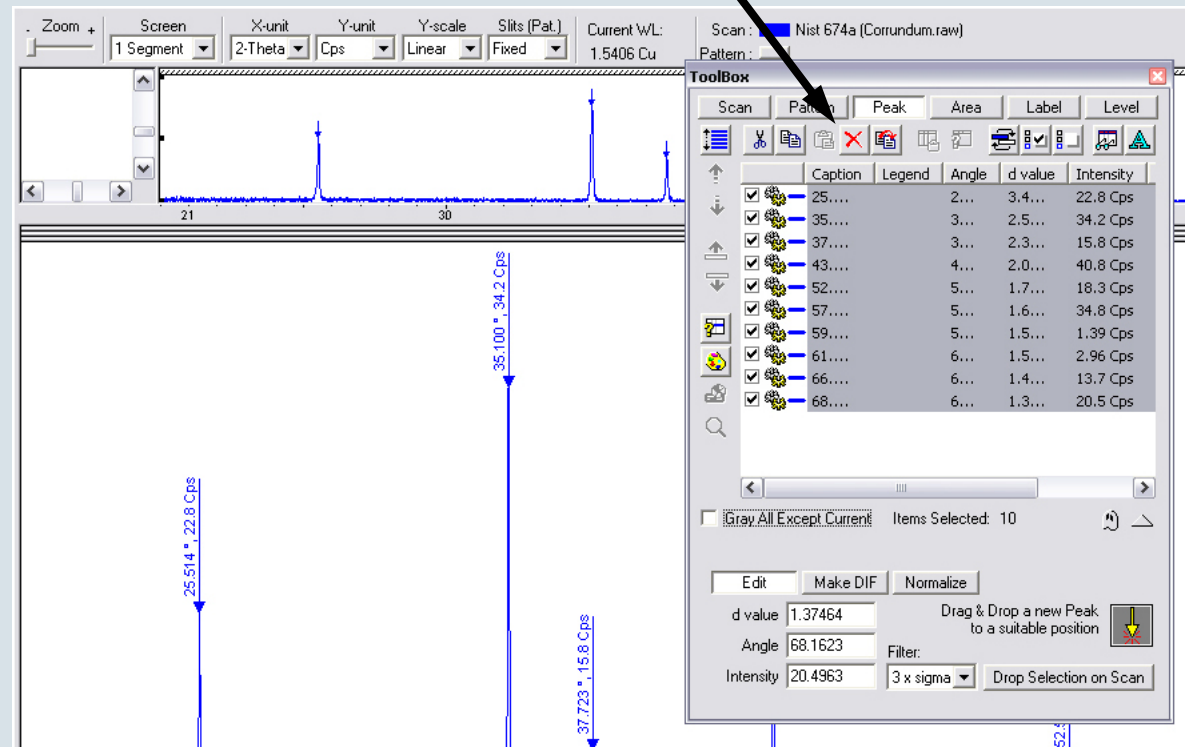
To change the default labels to **Angle, Intensity**:



1. Select **View > Settings**, then the **Sizes Tab**
2. Change the text box in the Peaks category from **d=%2** to **%1, %3**

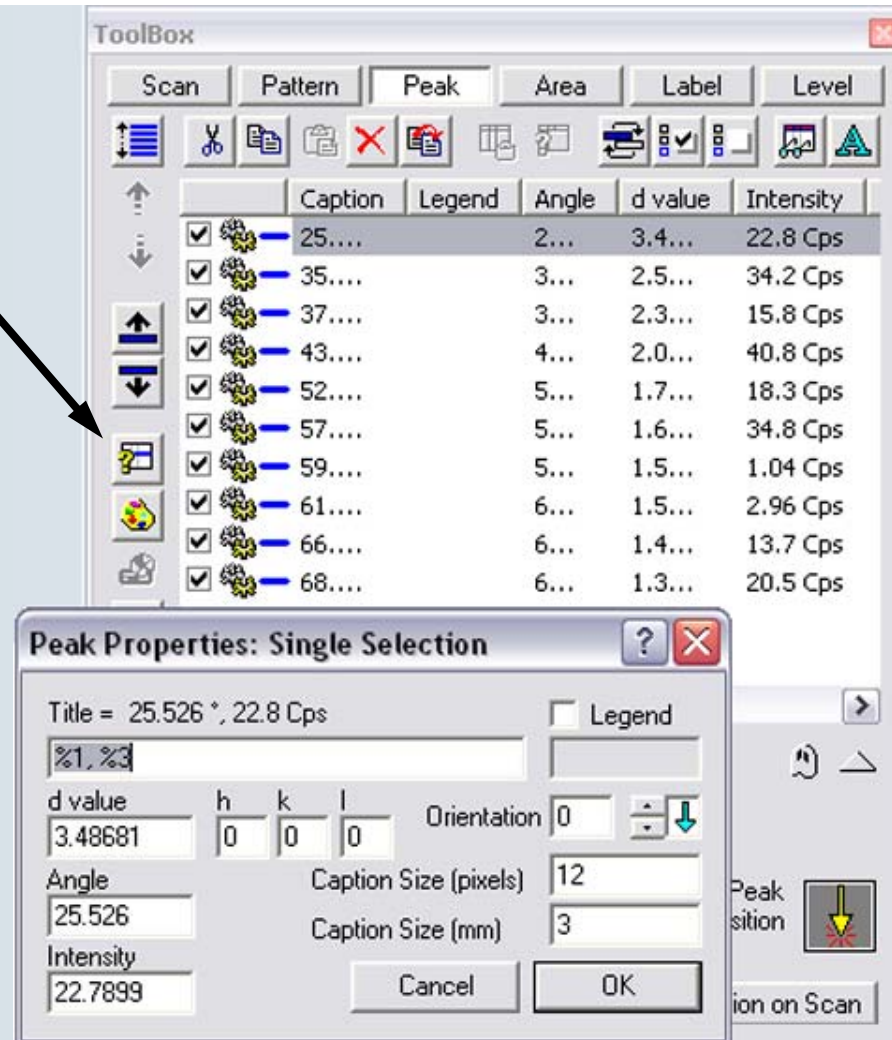
# Changing the Default Peak Label

3. Highlight the old peaks and select **X** to delete them
4. Redo the peak search on the scan tab and select **Append to List**



# Changing Individual Peak Properties

1. Highlight the peak
2. Select **Properties**



The screenshot shows the 'ToolBox' window with a list of peaks. The 'Peak' tab is selected. The peak list is as follows:

Caption	Legend	Angle	d value	Intensity
25....		2...	3.4...	22.8 Cps
35....		3...	2.5...	34.2 Cps
37....		3...	2.3...	15.8 Cps
43....		4...	2.0...	40.8 Cps
52....		5...	1.7...	18.3 Cps
57....		5...	1.6...	34.8 Cps
59....		5...	1.5...	1.04 Cps
61....		6...	1.5...	2.96 Cps
66....		6...	1.4...	13.7 Cps
68....		6...	1.3...	20.5 Cps

The 'Peak Properties: Single Selection' dialog box is open for the selected peak. The properties are:

- Title = 25.526 °, 22.8 Cps
- Legend:
- d value: 3.48681
- h: 0, k: 0, l: 0
- Orientation: 0
- Angle: 25.526
- Intensity: 22.7899
- Caption Size (pixels): 12
- Caption Size (mm): 3

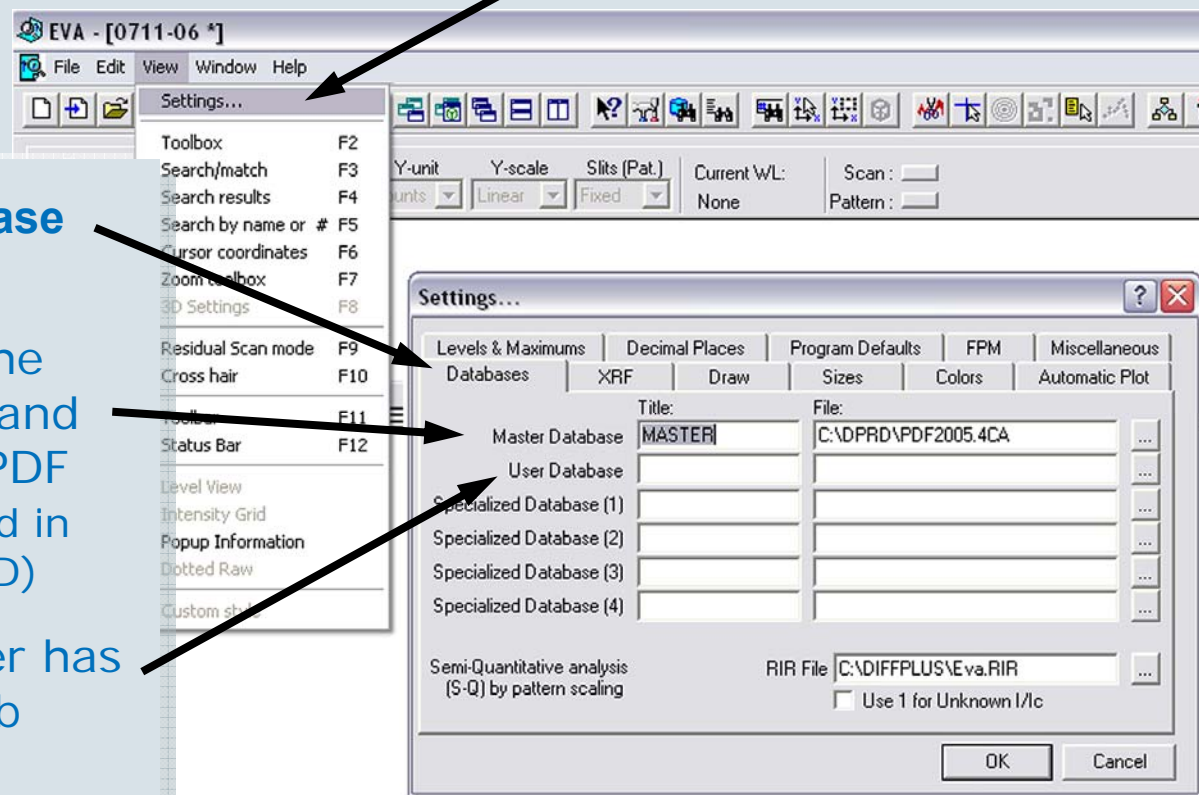
# Setting the Database Location

1. Open the **Settings** Palette: Select **View > Settings...**

2. Select the **Database** tab

3. Type a title for the **Master Database** and navigate to the PDF Db (Usually located in C:\ PDF or C:\DPRD)

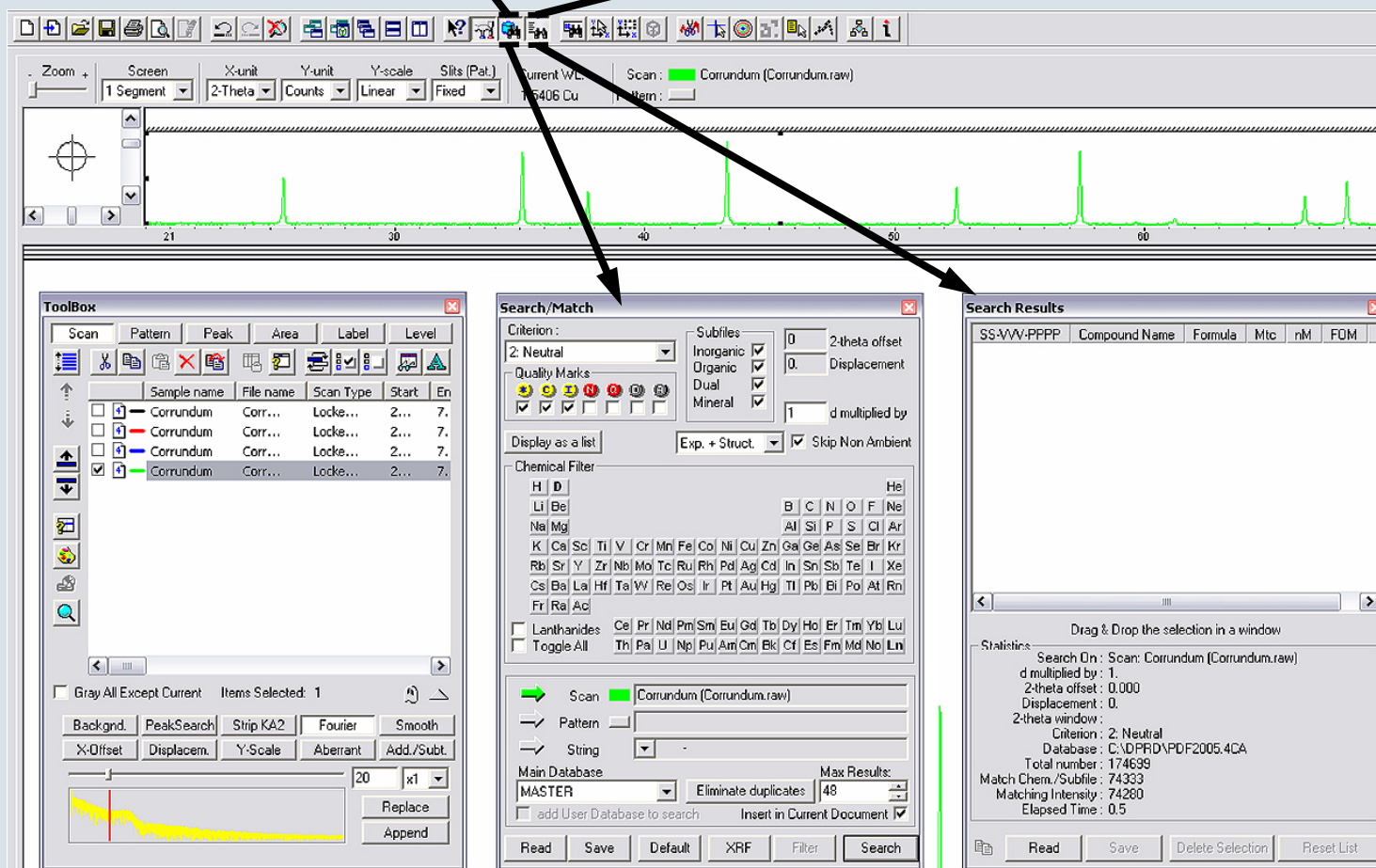
4. Repeat if the user has a custom user Db



# Opening the Search/ Match Windows

1. Open the Search/ Match window

2. Open the Search Results window



The screenshot displays the Bruker software interface with an XRD pattern at the top. Below the pattern are three windows:

- ToolBox:** A window with tabs for Scan, Pattern, Peak, Area, Label, and Level. It contains a table of scan data and various processing buttons.
- Search/Match:** A window for configuring search criteria. It includes a 'Criterion' dropdown set to '2: Neutral', 'Quality Marks' checkboxes, a 'Chemical Filter' grid, and a 'Scan' field containing 'Corundum (Corundum.raw)'. Buttons for 'Read', 'Save', 'Default', 'XRF', 'Filter', and 'Search' are at the bottom.
- Search Results:** A window showing search statistics and a table of results. The table has columns for 'SS-VVV-PPPP', 'Compound Name', 'Formula', 'Mtc', 'nM', and 'FOM'. The statistics section shows: Search On: Scan: Corundum (Corundum.raw), d multiplied by: 1, 2-theta offset: 0.000, Displacement: 0, 2-theta window: Criterion: 2: Neutral, Database: C:\DPRD\PDF2005.4CA, Total number: 174699, Match Chem./Subfile: 74333, Matching Intensity: 74260, Elapsed Time: 0.5.



# Search/ Match Window

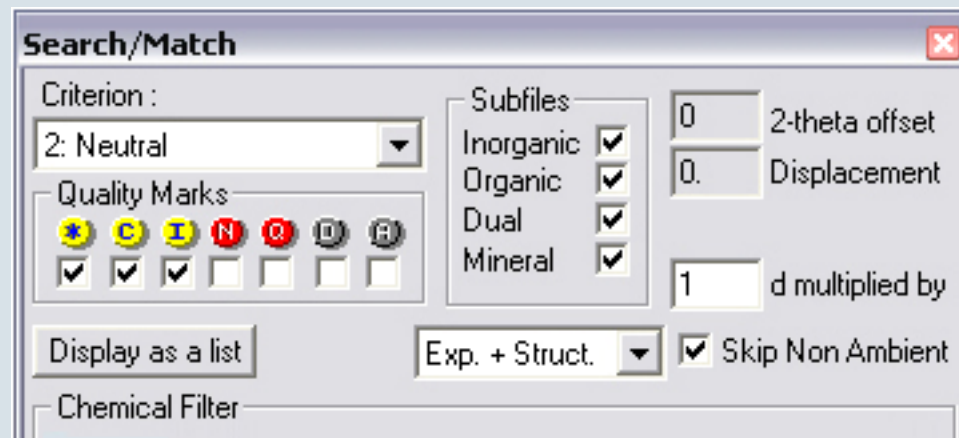
## ■ Criterion:

- Favor Simple Patterns - Patterns with the least matching peaks
- Neutral - Usual Setting; no preference
- Favor Complex Patterns - Patterns with the most matching peaks

## ■ Subfiles: Which subdatabases should be included

## ■ Quality Marks

- Yellow are the most reliable
- Red indicates the pattern is missing some information
- Grey are not reliable



## ■ Experimental/ Structural

- Experimental: ICDD patterns
- Structure: Patterns calculated from the structure Db

## ■ Skip Non Ambient - Skip patterns where the measurement was not carried out at room temperature / pressure

# Search/ Match Window (continued)

- Chemical Filter - Click the element to change its color
  - Red = not present
  - Grey = might be present
  - Green = must be present
  - Toggle all will change all of the elements' colors
- Scan
  - The scan which will be searched
- Eliminate Duplicates
  - If 2 patterns had the exact same name and line positions, it will eliminate them from the results

**Chemical Filter**

H	D																	He
Li	Be											B	C	N	O	F	Ne	
Na	Mg											Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	Ac																
<input type="checkbox"/> Lanthanides		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
<input type="checkbox"/> Toggle All		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Ln			

Scan Corrundum (Corrundum.raw)

Pattern

String

Main Database: MASTER
Eliminate duplicates
Max Results: 48

add User Database to search
  Insert in Current Document

Read
Save
Default
XRF
Filter
Search



# Performing a Search/ Match

1. Highlight the last scan on the list. This scan had the background subtracted,  $K_{\alpha 2}$  stripped, and Fourier smoothing applied

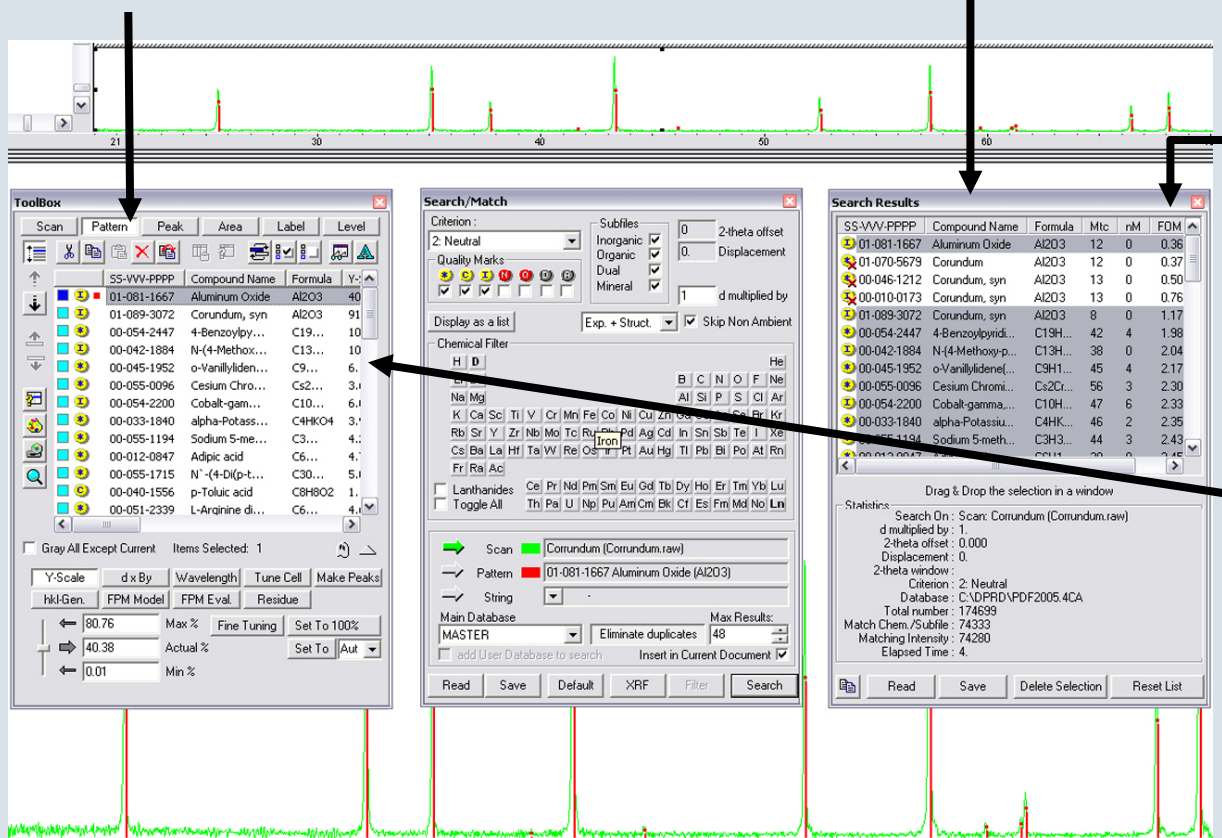
The image shows two overlapping software windows. The 'ToolBox' window on the left displays a list of scans. The last scan, 'Corrundum Corr... Lock... 2... 7.', is highlighted. Below the list are buttons for 'Backgnd.', 'PeakSearch', 'Strip KA2', 'Fourier', and 'Smooth', along with a small XRD plot. The 'Search/Match' window on the right has the following settings:

- Criterion: 2: Neutral
- Quality Marks: Inorganic, Organic, Dual, Mineral (all checked)
- Subfiles: 0 (2-theta offset), 0 (Displacement), 1 (d multiplied by)
- Display as a list: Exp. + Struct. (selected), Skip Non Ambient (checked)
- Chemical Filter: H, D, He (checked)
- Buttons: Scan (green), Pattern, String
- Main Database: MASTER, Max Results: 48
- Buttons: Read, Save, Default, XRF, Filter, Search

2. Input the appropriate settings
3. If a user database is present, check this box
4. Select **Search**

# Search / Match Results

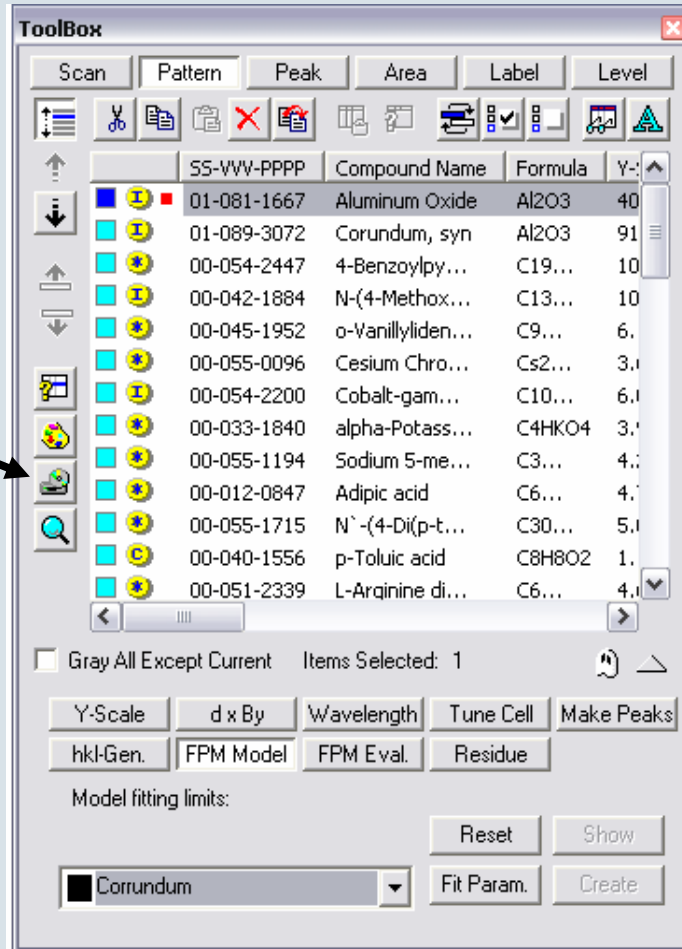
- Results are displayed in the **Search Results** window and the **Toolbox: Pattern** window



- The **Figure of Merit (FOM)** column gives a rough idea of how well the pattern matches. The lower the number, the better the match
- Highlighting a pattern shows the lines in the scan window

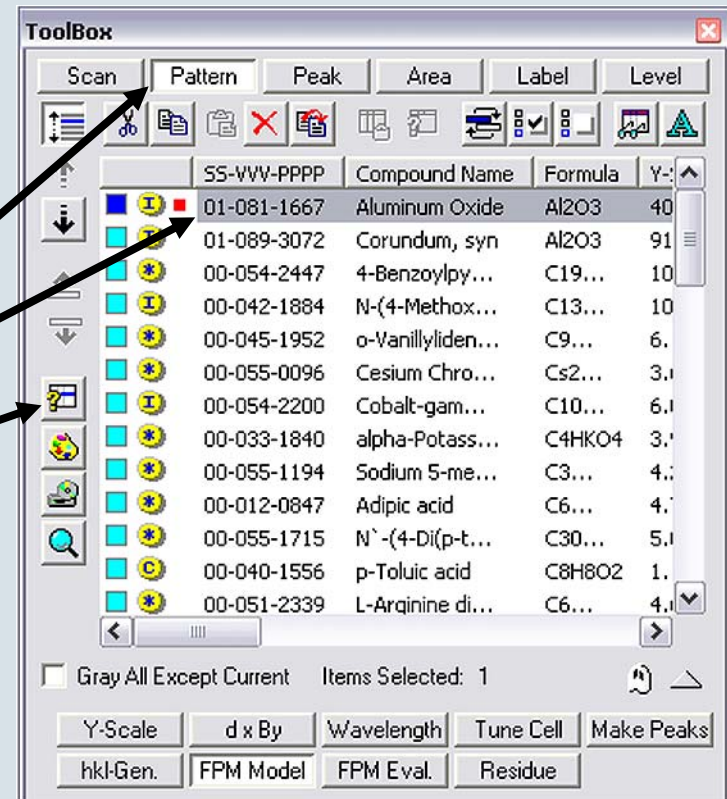
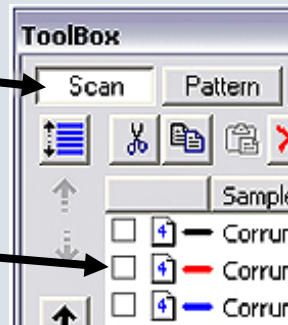
# Displaying the PDF for a Pattern

- Select the **PDF Database** button to view the PDF



# Refining Lattice Parameters

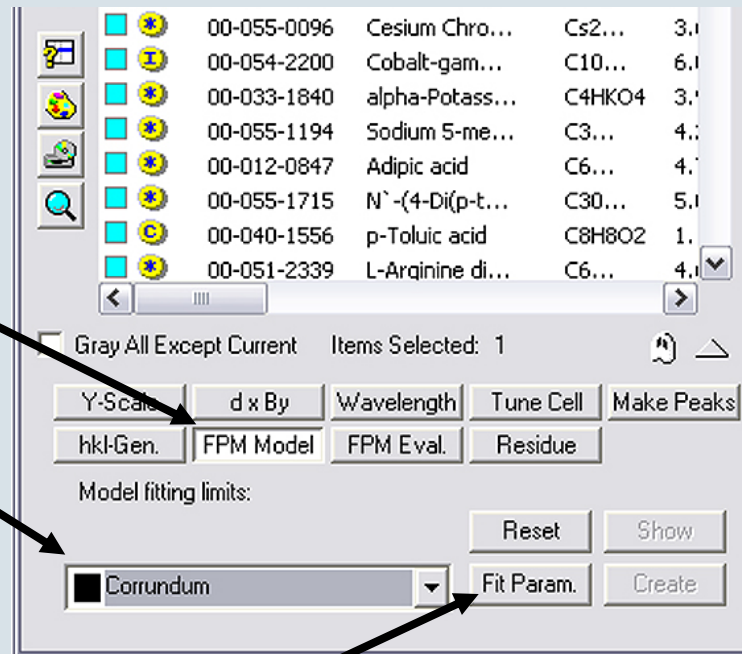
1. Navigate to the **Toolbox: Scan** window
2. Check the box next to the original scan so it is not hidden
3. Return to the **Toolbox: Pattern** window
4. Highlight the pattern that fits the scan the best
5. Select the **Properties** button and check the **FPM boxes**



# Lattice Parameter Refinement (continued)

6. Select **FPM Model**  
(**FPM Model** is refining a single phase, and **FPM Eval.** is for quantitatively refining a mixture)

7. Select the original scan file



8. Select **Fit Param.**, and the **Model Parameters** dialog will pop-up

9. In **Model Parameters** make sure none of the **Fixed** boxes are checked and select **OK**

# Lattice Parameter Refinement Result

- R/R0 is a measure of the fit, 1 is a perfect R/R0
- Approximate crystal (grain) size
- Refined lattice parameters

**FPM Fit results**

Number of steps:	20	
R/R0:	1.22	
RWP:	5.97	
Delta displacement:	-0.083	mm
01-081-1667 Aluminum Oxide		
----- Al <sub>2</sub> O <sub>3</sub>		
FWHM(30):	0.0851	°
Crystallite Size (Scherrer):	956.0	Å
System:	Rhombo.H.axes	
Space group:	R-3c (167)	
Cell param.:	Initial	Final
a:	4.76000	4.75976
c:	12.99300	12.99386

You need to hit the [Create] button in the tool to save this Fit result as a new MODEL scan.

Clipboard Copy    OK



