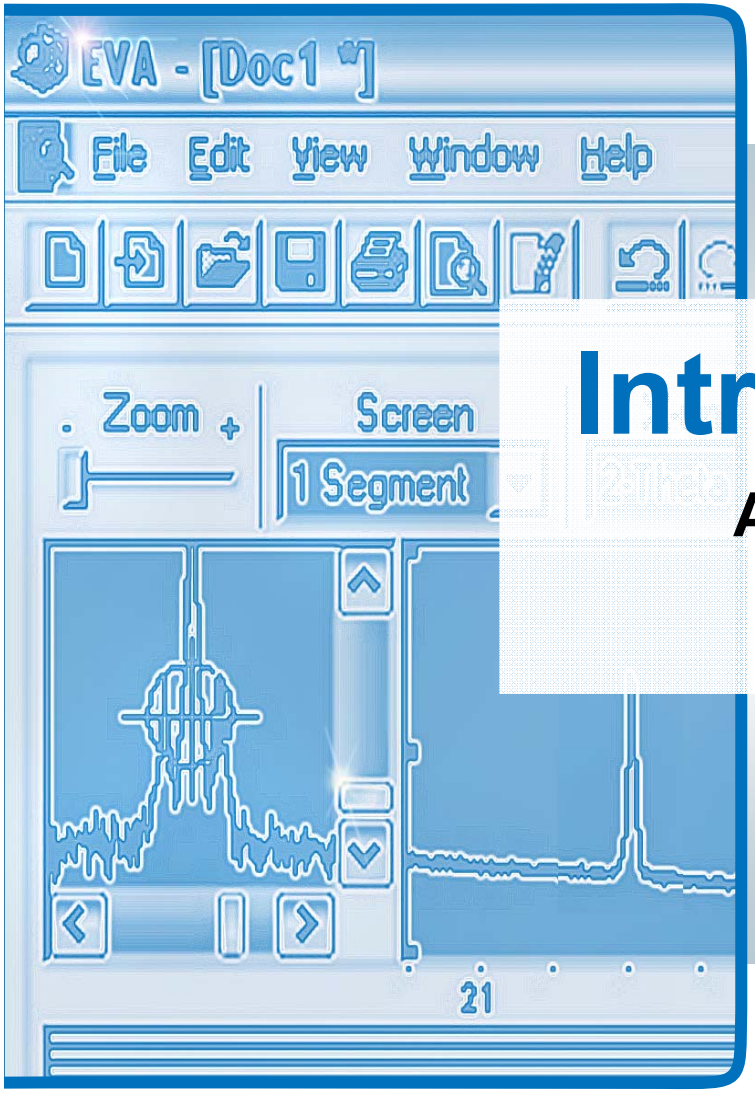
Bruker AXS



Introduction to EVA

A Complete Orientation to Features and Functions

Jonathan Giencke
Application Engineer, X-ray Diffraction

Overview

Bruker AXS

1. Introduction
2. Layout of EVA
3. Importing a Scan
4. Zooming on a Scan Range
5. Stripping $K_{\alpha 2}$
6. Determining the FWHM and Position of Peaks Using the Area Function
7. Subtracting the Background
8. Cleaning up the Worksheet
9. Smoothing the Scan (to reduce noise)
10. Extra Toolbox functions
11. Peak Search, Labeling Peaks and Making a DIF
12. Performing a Search / Match
13. Refining Lattice Parameters

Introduction

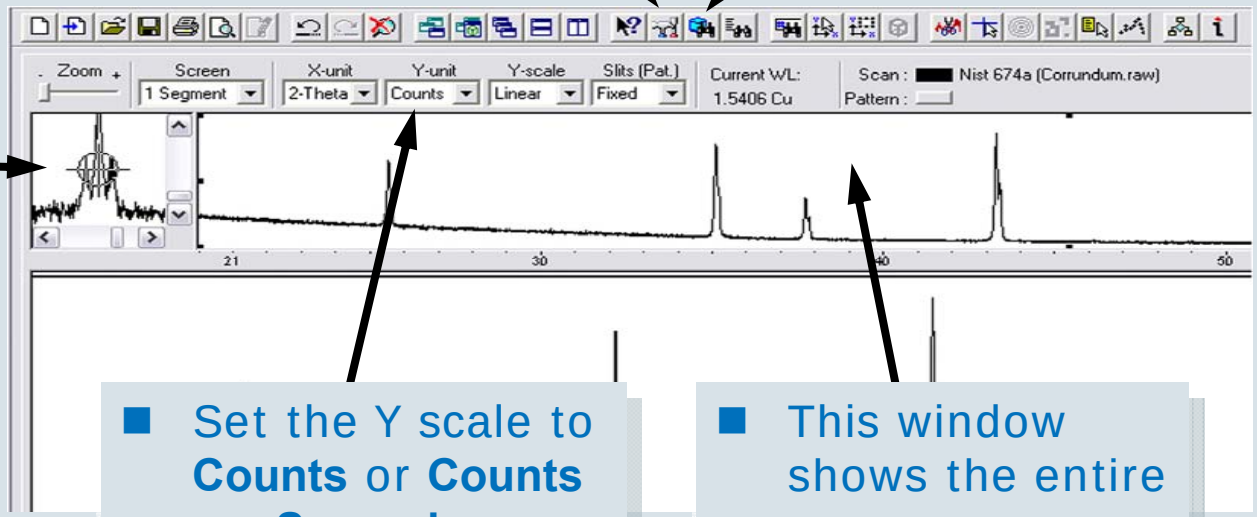
Bruker AXS

- 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)

Bruker AXS

- Toolbox
- Search/ Match
- Magnified view of the cursor location

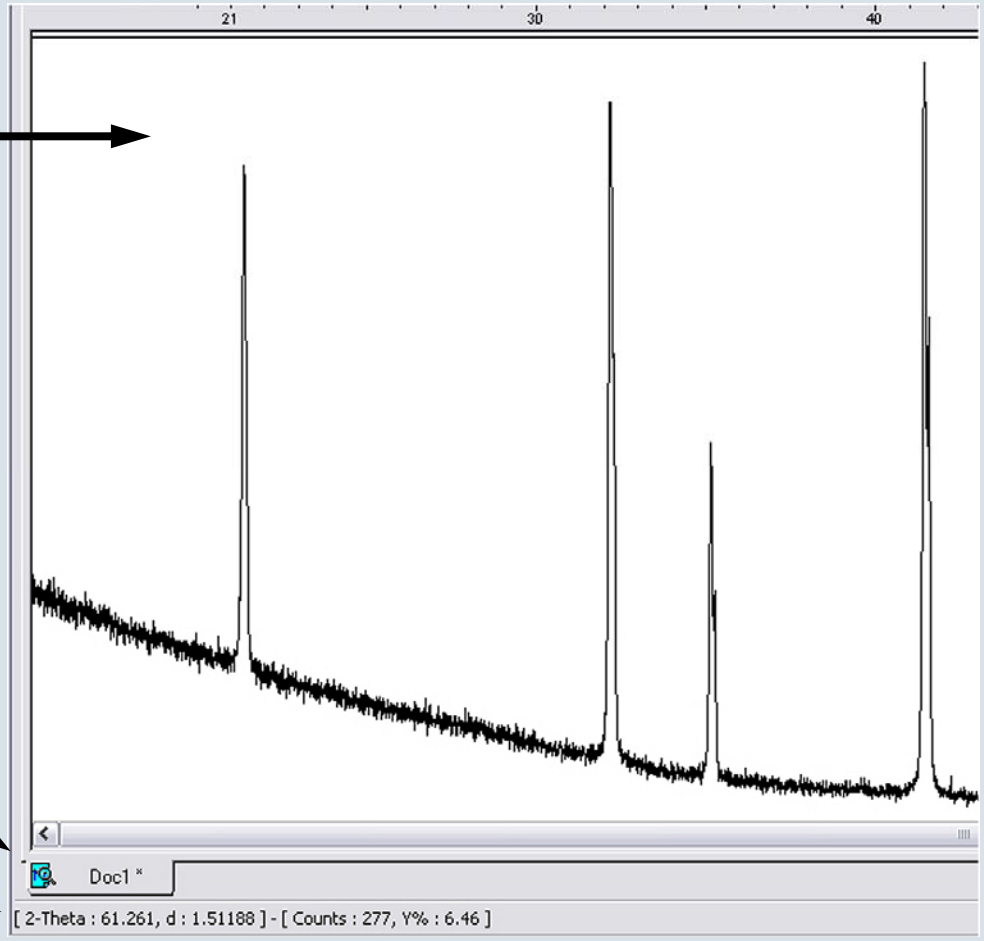


- Set the Y scale to **Counts** or **Counts per Second**
- This window shows the entire scan

Layout of EVA
(lower portion)

Bruker AXS

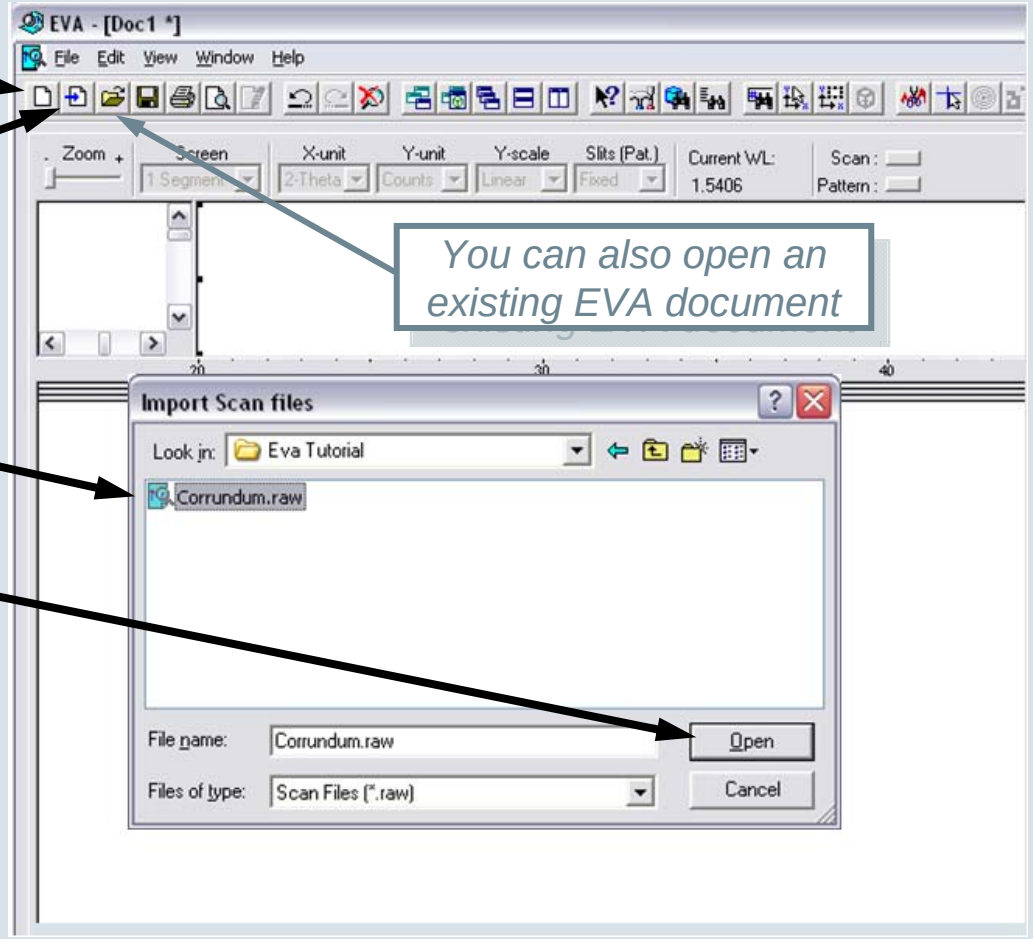
- Main editing window
- Worksheet tabs
- Position of the cursor (coordinates)



Importing a Scan

Bruker AXS

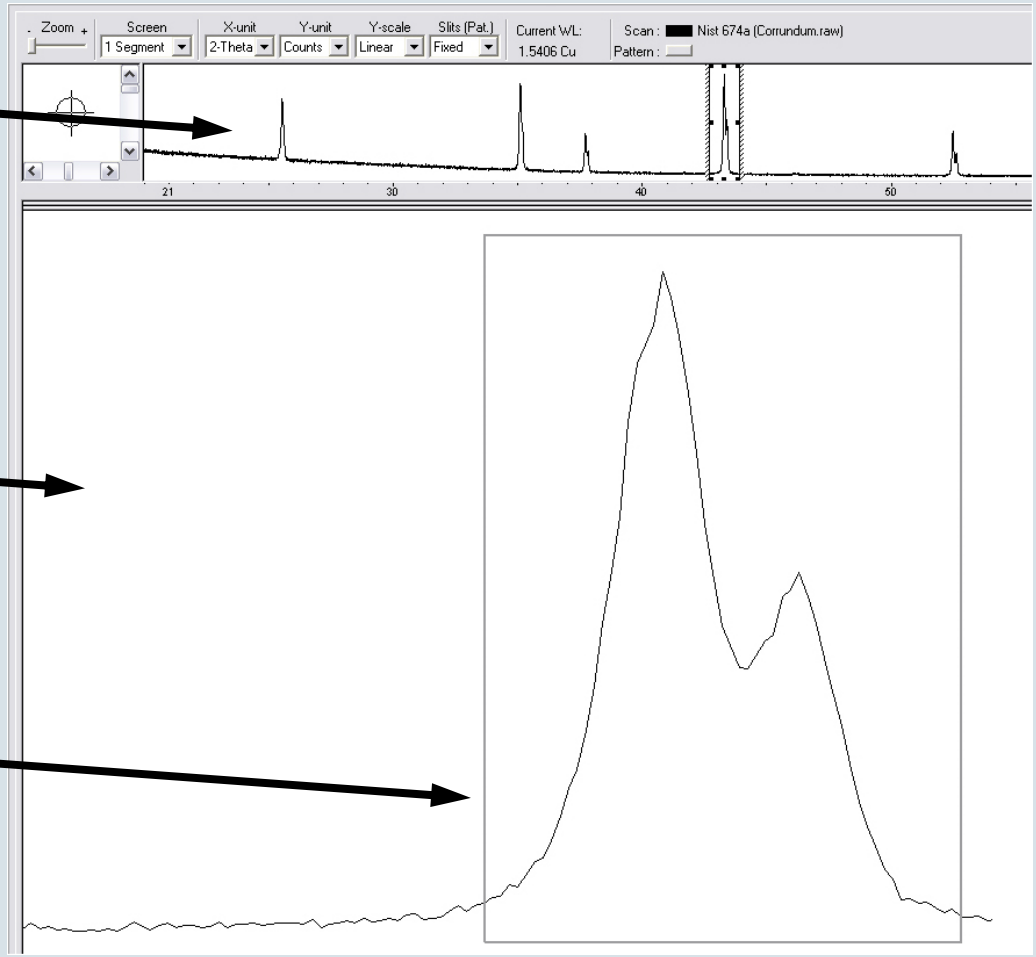
1. Select **New Worksheet**
2. Select **Import a scan** (.raw file) button
3. Select a scan with a mouse-click. To import multiple scans, press the [Ctrl] key while clicking
4. Select **Open**



Zooming on a Scan Range

Bruker AXS

- 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

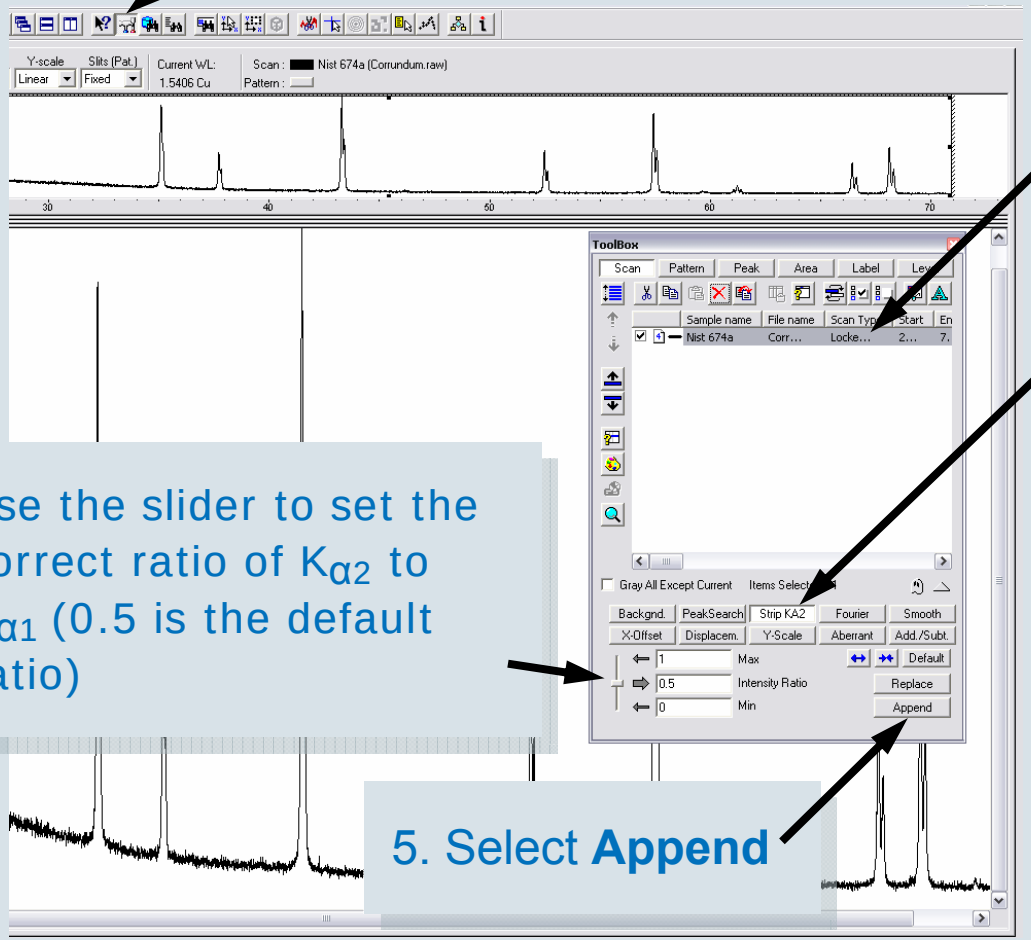


Stripping $K_{\alpha 2}$

(Applicable to machines that do not have a monochromator)

Bruker AXS

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)

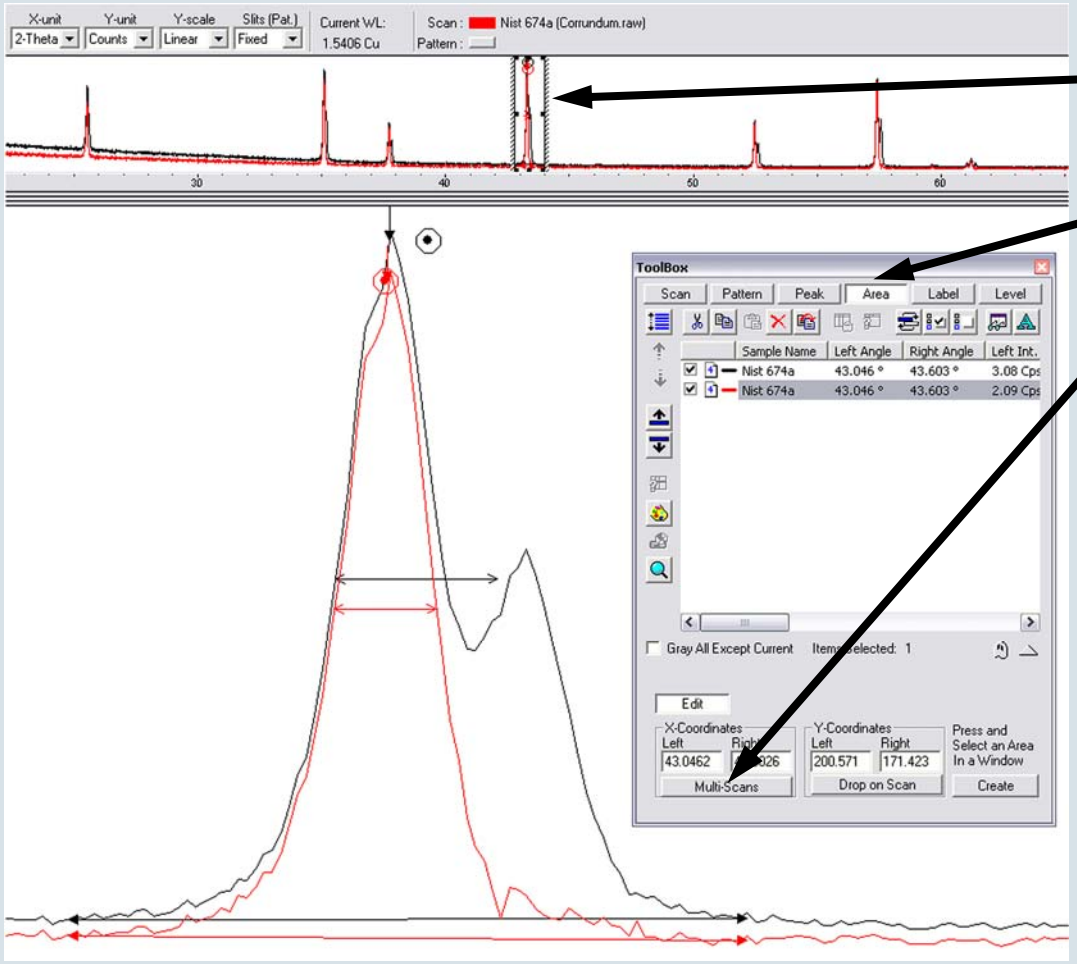
5. Select **Append**

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

Bruker AXS

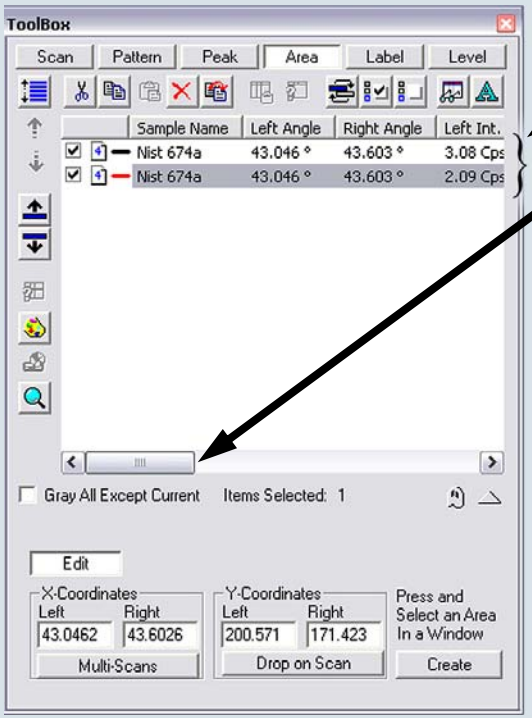


1. Zoom in on a peak
2. Select the **Area** tab in the **Toolbox**
3. Select **Multi-Scans**
4. Select **Create**
5. Using the mouse, drag a region over the peak

*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)

Bruker AXS



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*

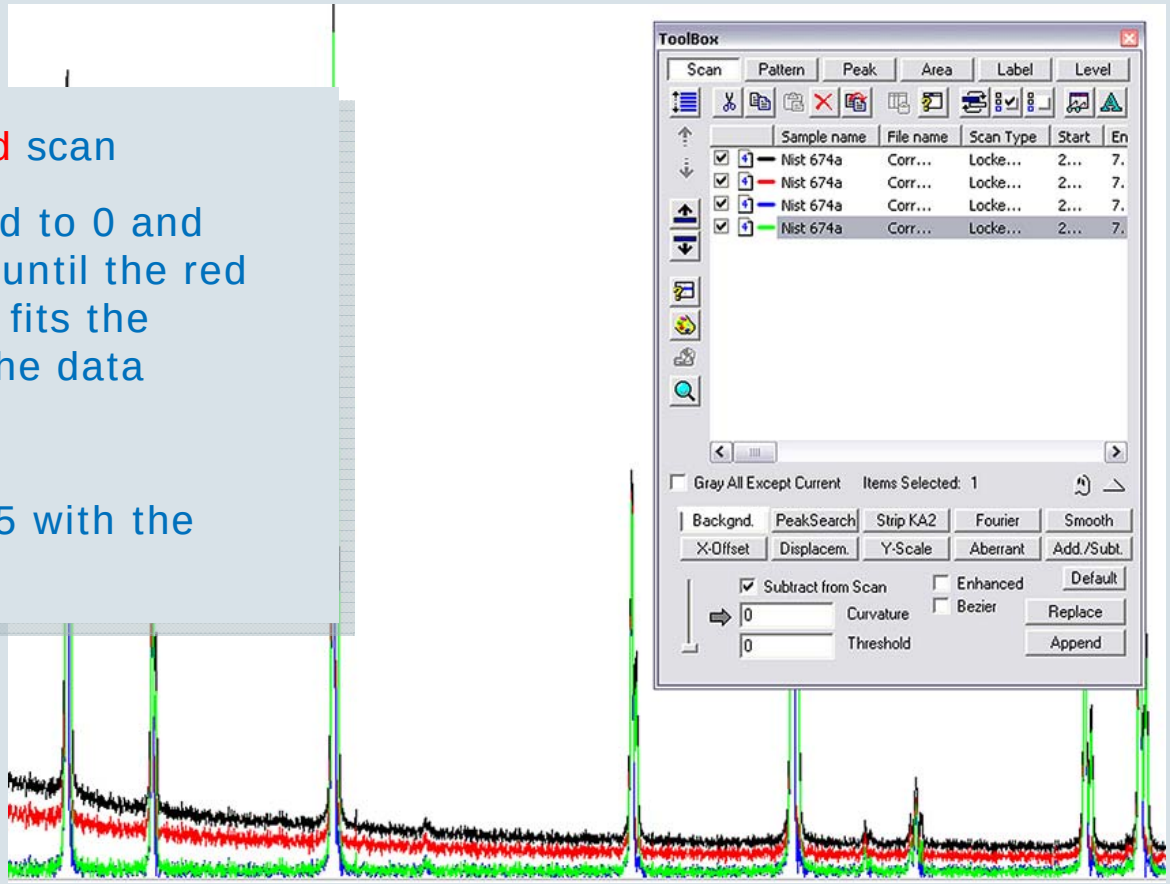
Note that **Gravity Center**, **Chord Mid** and **FWHM** are only valid for isolated peaks!

Subtracting the Background

In preparation for doing a Search / Match

Bruker AXS

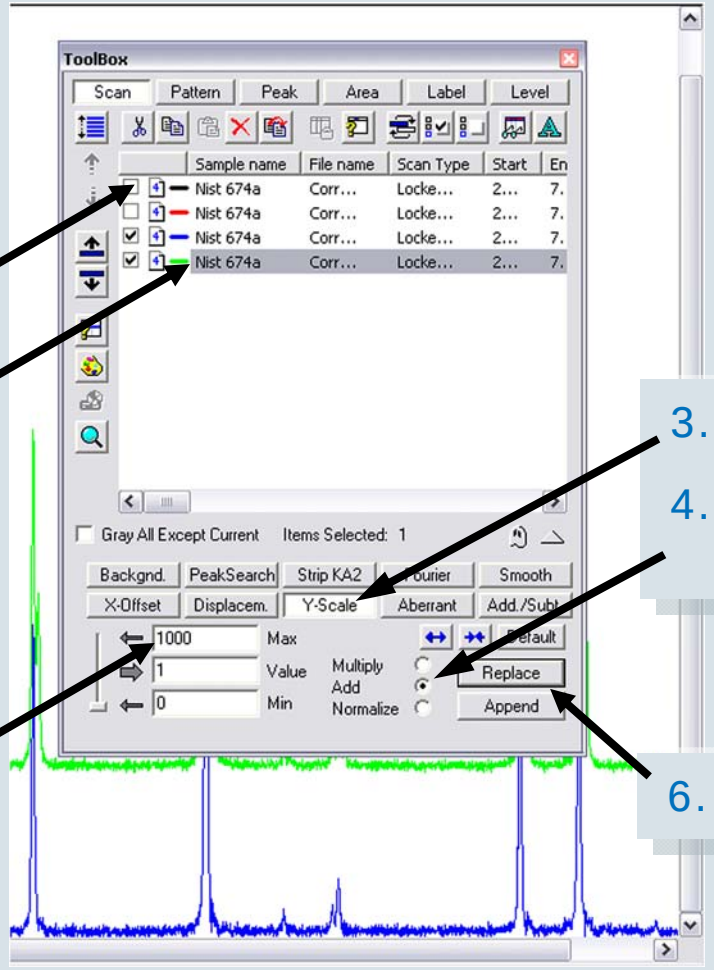
1. Highlight the red scan
2. Set the threshold to 0 and move the slider until the red background line fits the background of the data
3. Select **Append**
4. Repeat steps 1-5 with the black scan



Cleaning Up the Worksheet

Bruker AXS

1. Hide the “non background subtracted” scans by double clicking the checkbox
2. Highlight the pre-$K_{\alpha 2}$ stripping scan

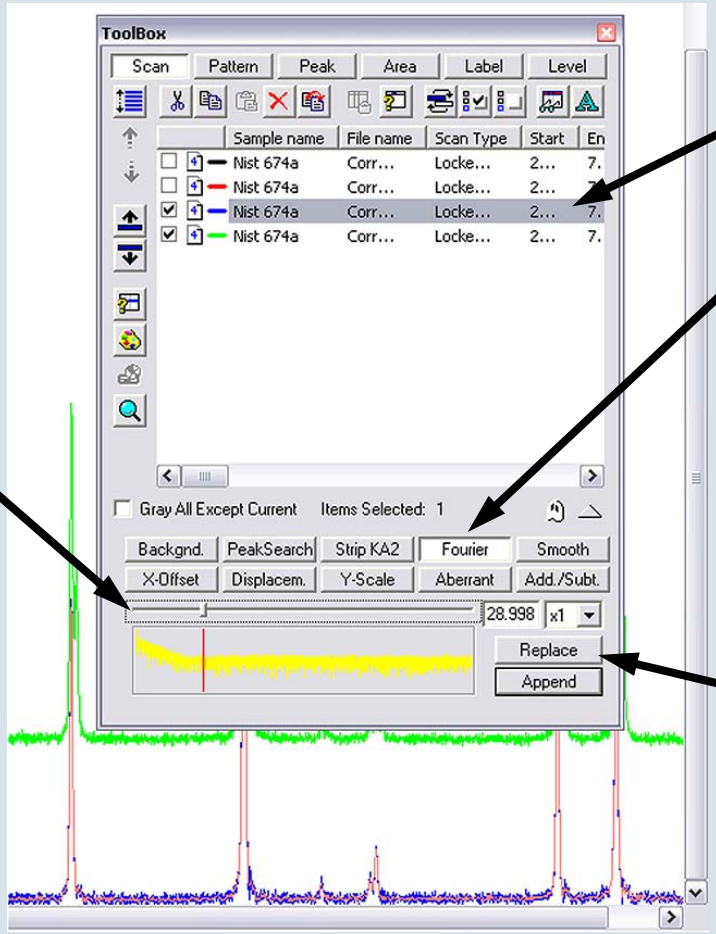


3. Select **Y-Scale**
4. Check the **Add** circle
5. Set **Max** to ¼ the intensity of the highest peak and **Min** to 0. Then using the slide translate the scan vertically
6. Select **Replace**

Smoothing the Scan

If the scan has an unacceptable amount of noise

Bruker AXS

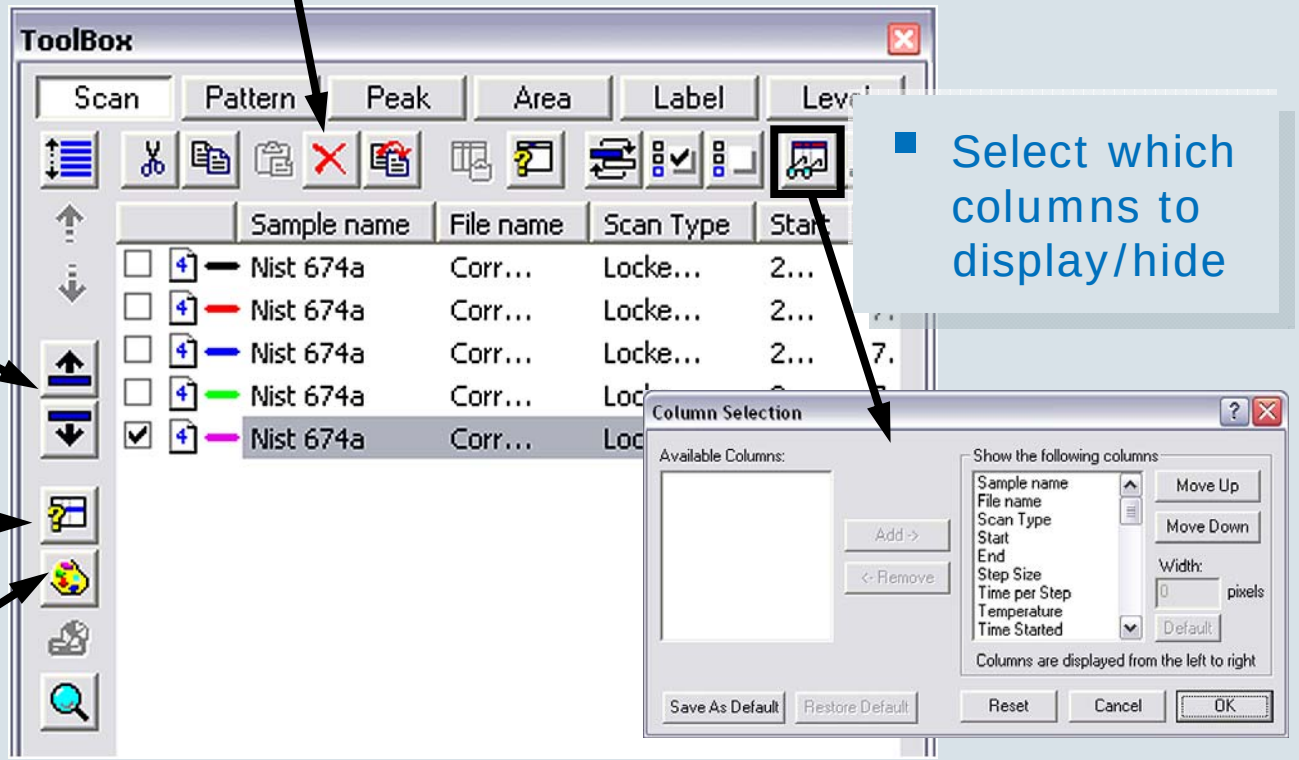


1. Highlight the Scan with $K_{\alpha 2}$ subtracted
2. Select **Fourier** (You could also try **Smooth** but we have gotten better results with **Fourier)**
3. Use the slider to set the red line on the right side of the bend
4. Select **Replace**

Additional Toolbox Functions

Bruker AXS

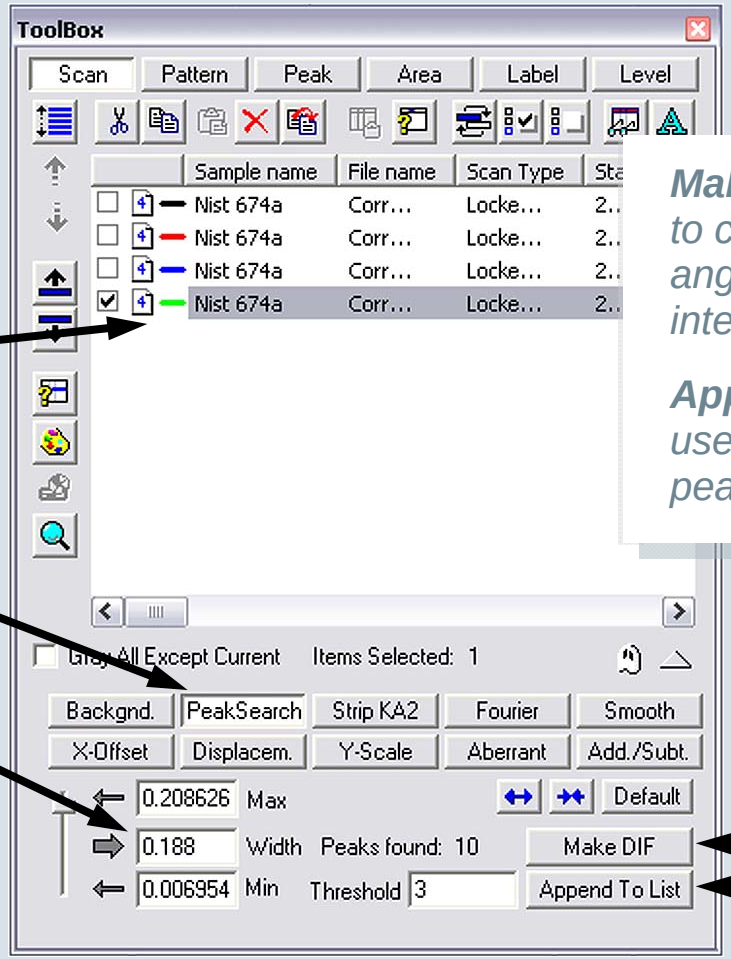
- Delete the highlighted scan
- Move the scan up or down in the list
- Various properties of the scan
- Change the color of the scan
- Select which columns to display/hide



Peak Search

Bruker AXS

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*

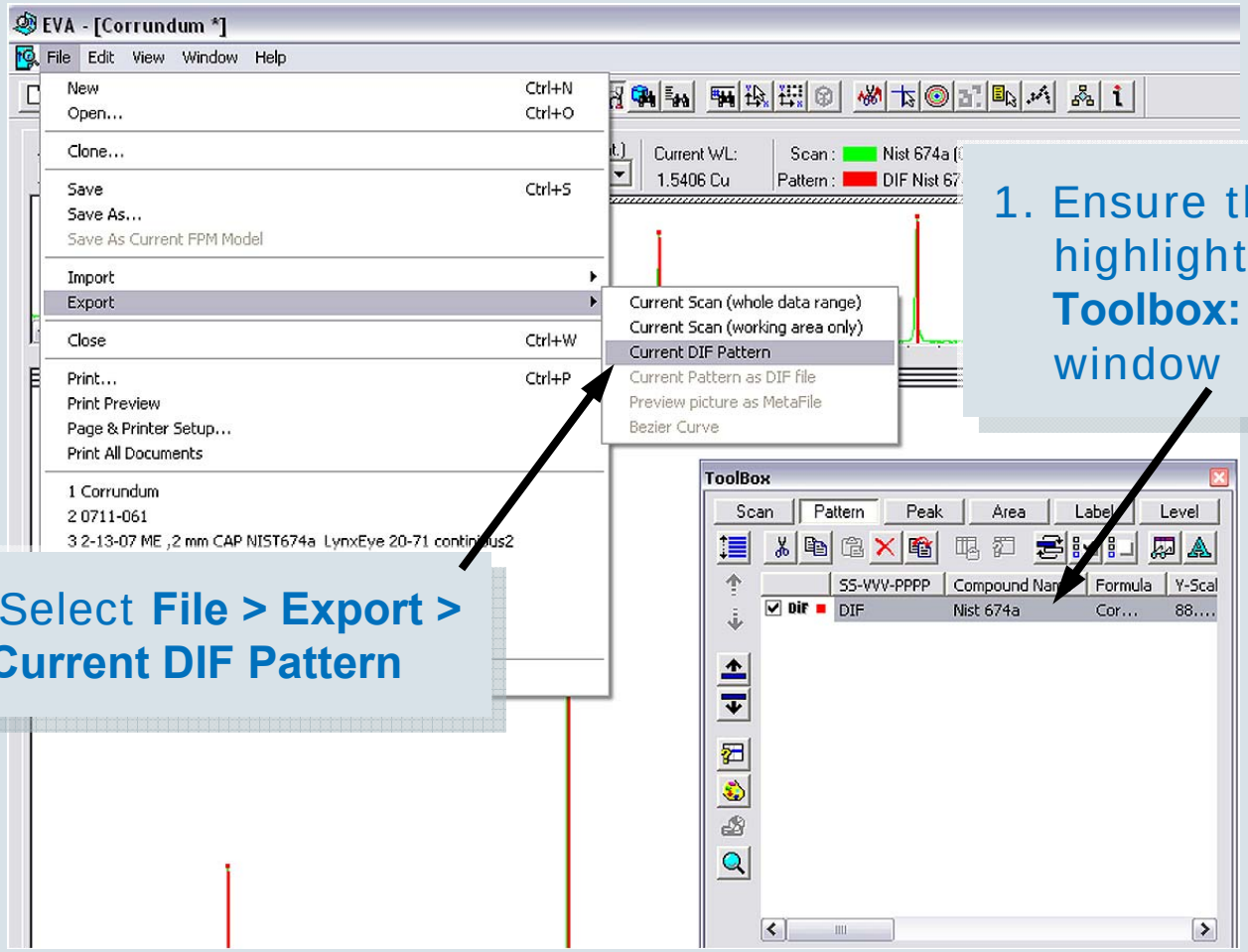
Append to List *is used to label the peaks in a scan*

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

Peak Search - Exporting the DIF

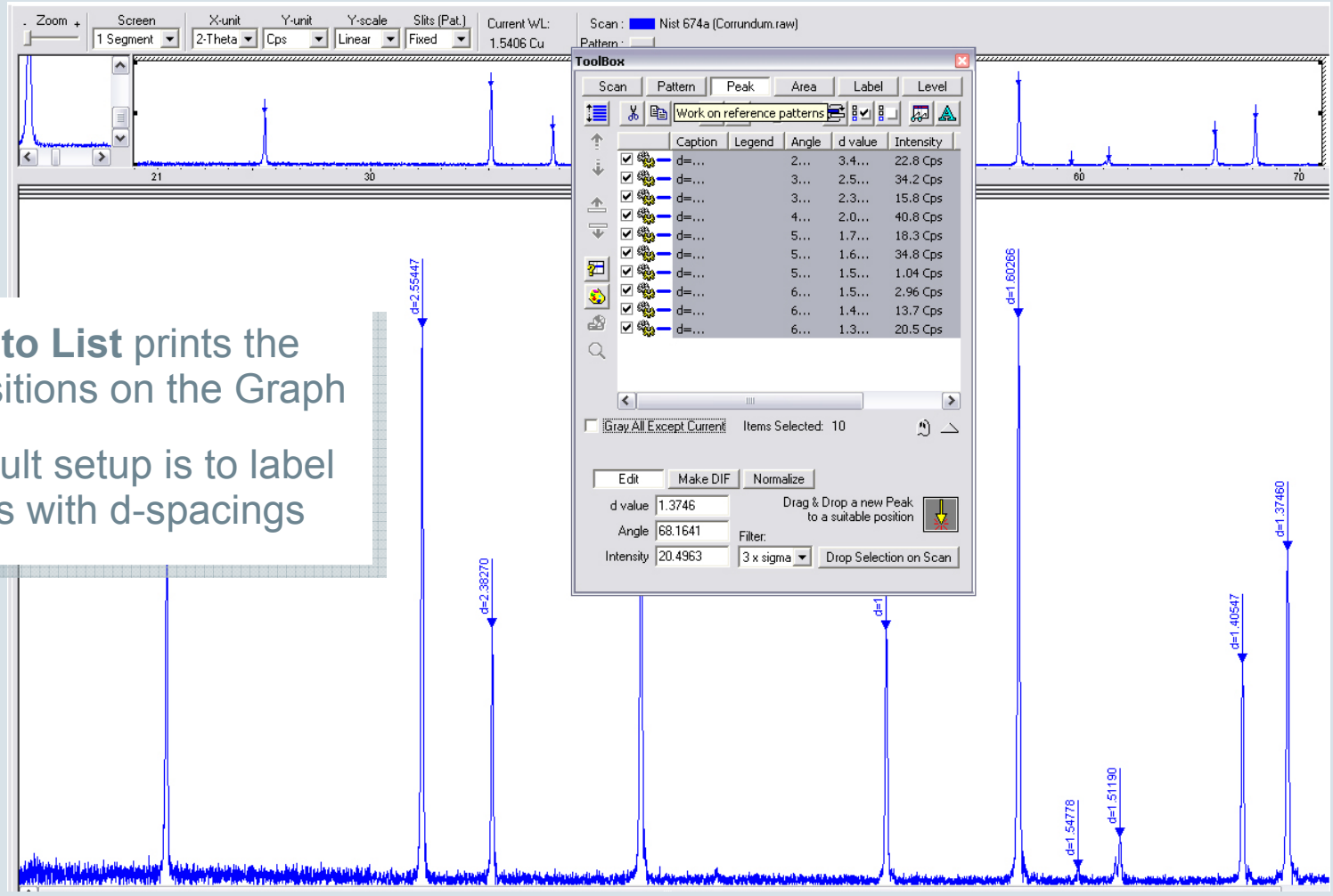
(Used to create custom patterns in a PDF Db)

Bruker AXS



Peak Search - Append to List

Bruker AXS



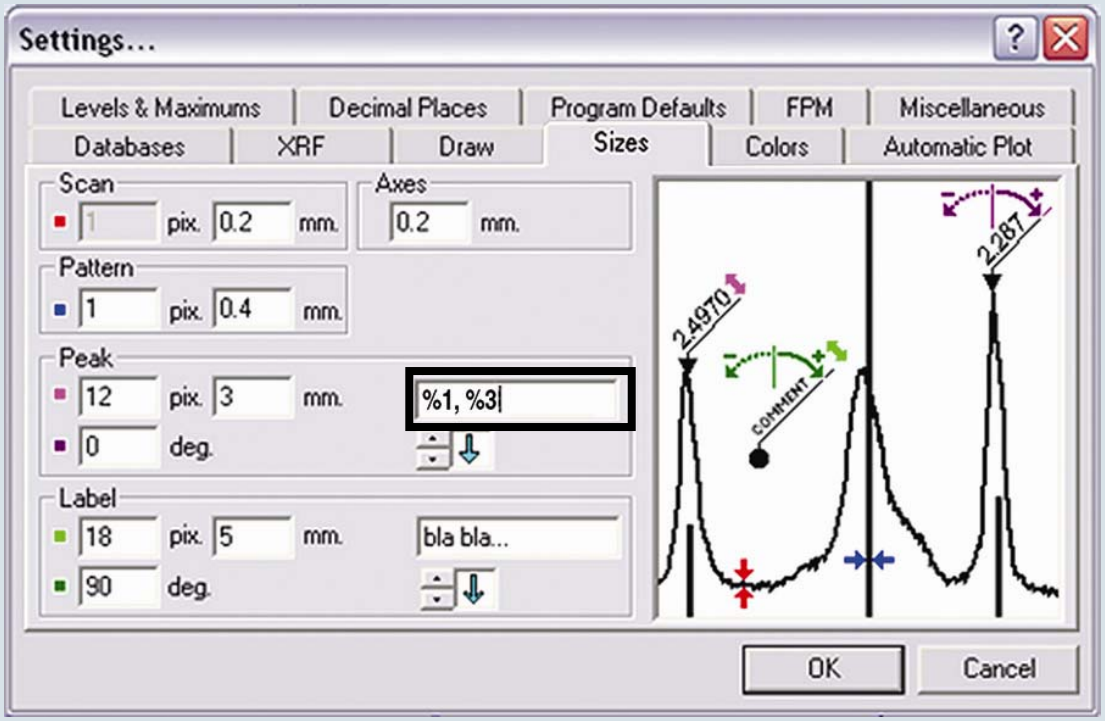
Append to List prints the peak positions on the Graph

The default setup is to label the peaks with d-spacings

Changing the Default Peak Label

Bruker AXS

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

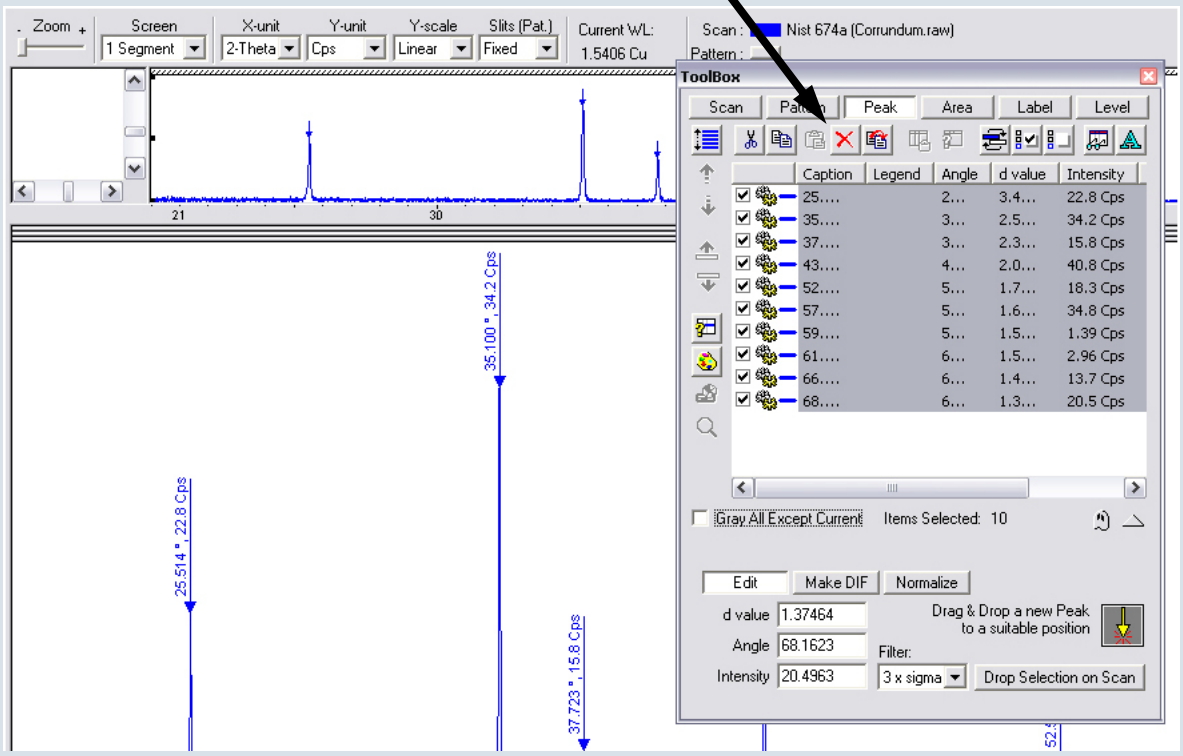


1. Select **View> Settings,** then the **Sizes Tab**
2. Change the text box in the Peaks category from **d=%2** to **%1, %3**

Changing the Default Peak Label

3. Highlight the old peaks and select **X** to delete them

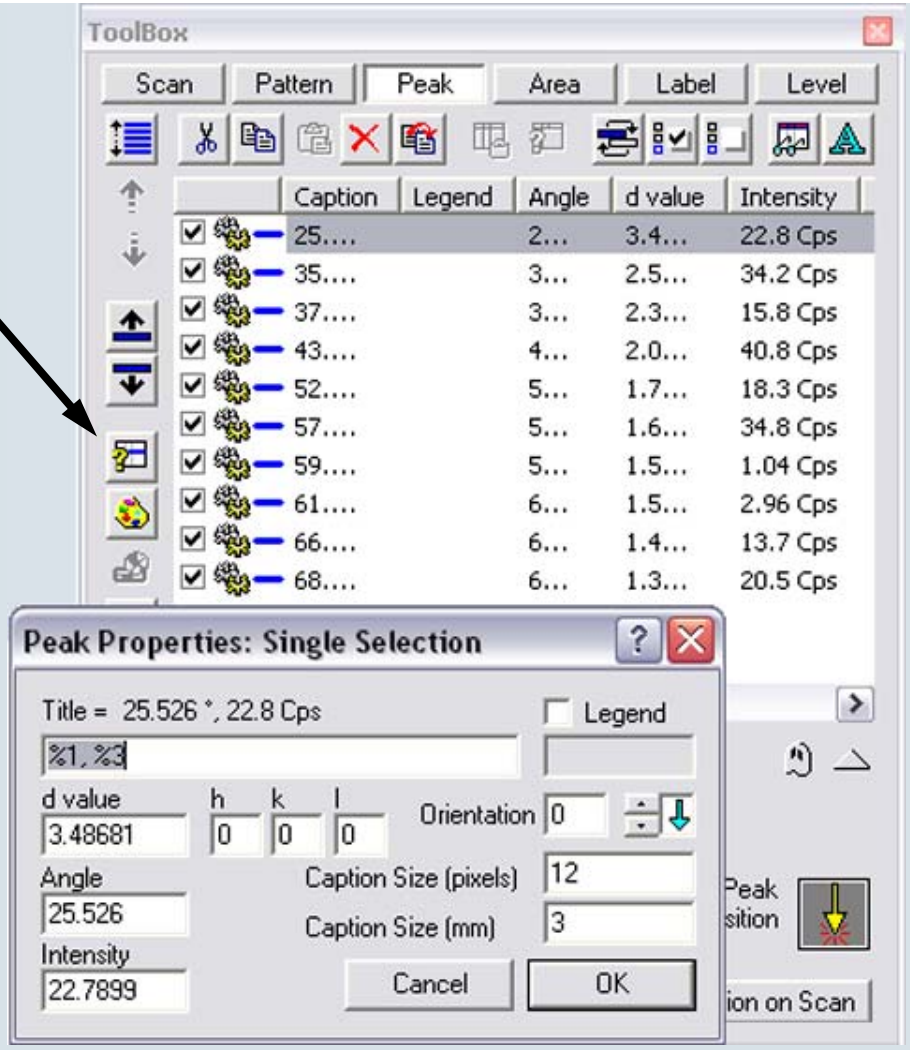
4. Redo the peak search on the scan tab and select **Append to List**



Changing Individual Peak Properties

Bruker AXS

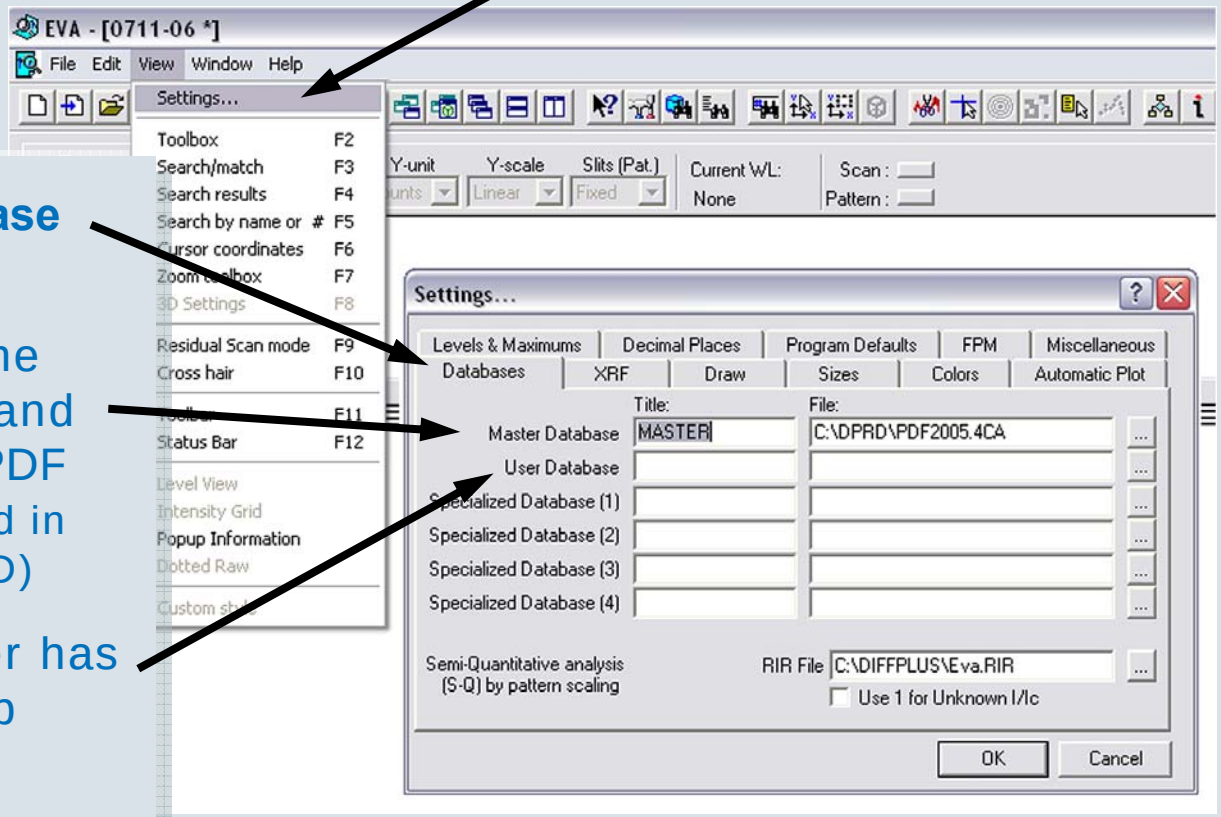
1. Highlight the peak
2. Select **Properties**



Setting the Database Location

Bruker AXS

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



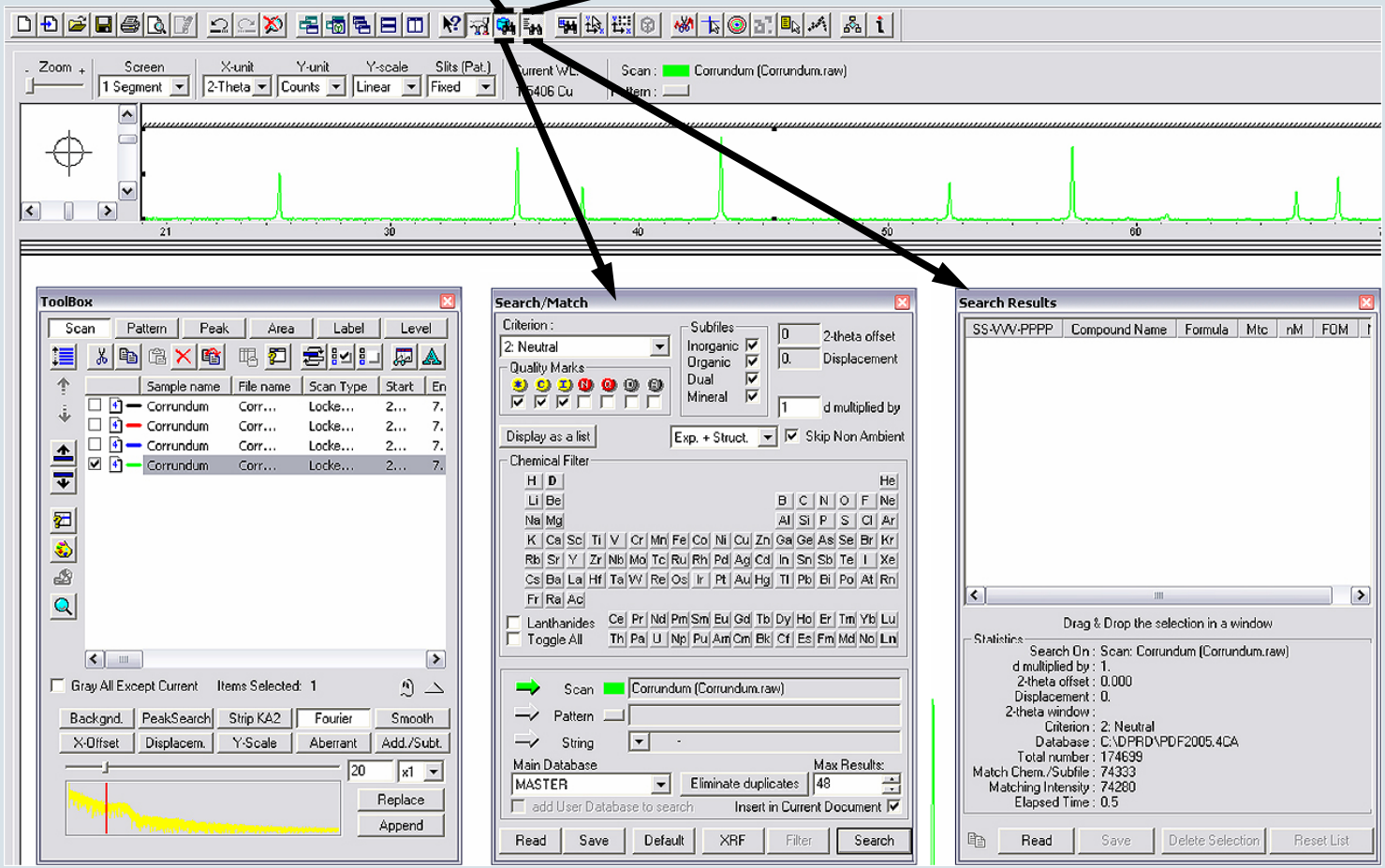
2. Select the **Database** tab
3. Type a title for the **Master Database** and navigate to the PDF Db (Usually located in C:\ PDF or C:\DPRD)
4. Repeat if the user has a custom user Db

Opening the Search/ Match Windows

Bruker AXS

1. Open the Search/ Match window

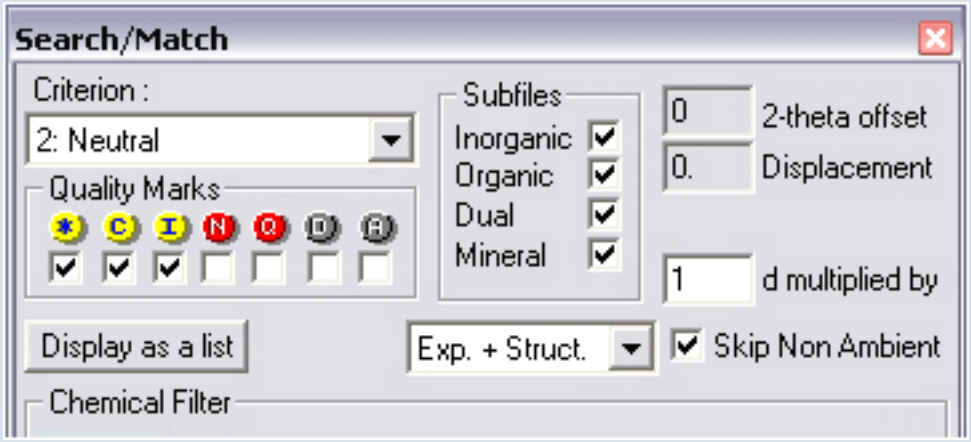
2. Open the Search Results window



Search/ Match Window

Bruker AXS

- 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

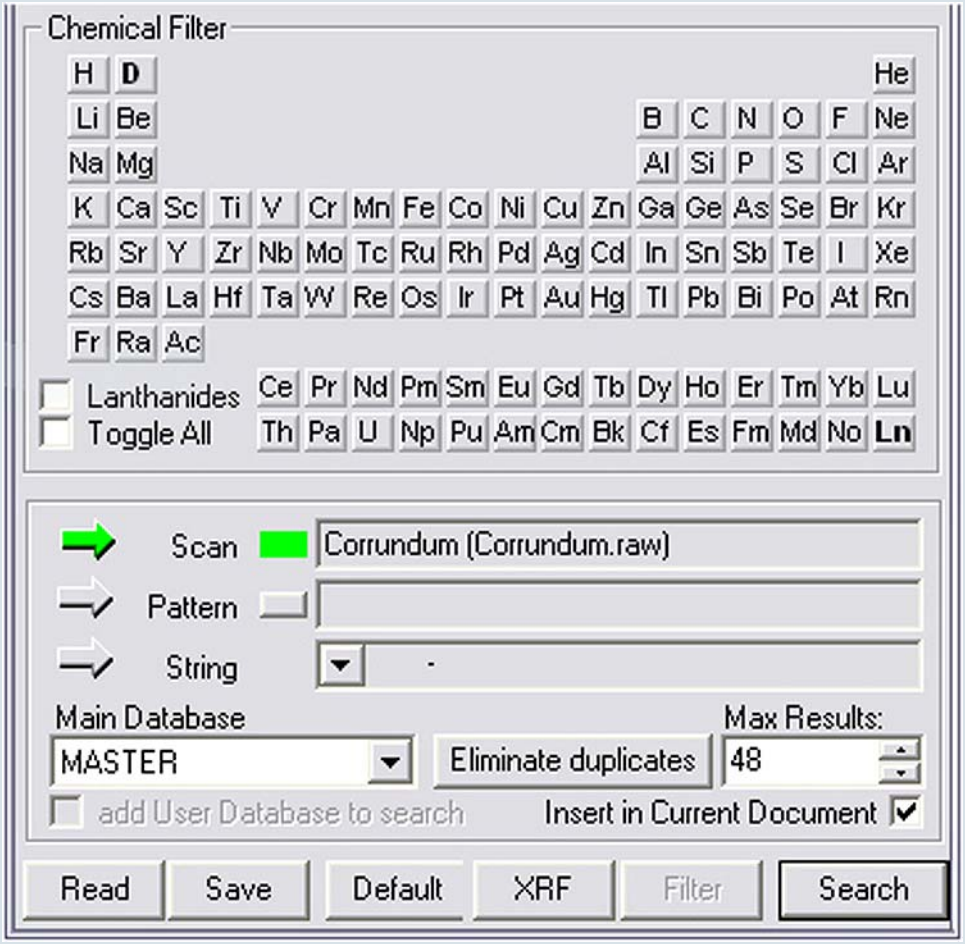


- Experimental/ Structural
  - Experimental: ICDD patterns
  - Structure: Patterns calculated from the structure Db
- Skip Non Ambient - Skip patterns where the measurement was not carried out at room temperature / pressure

Search/ Match Window
(continued)

Bruker AXS

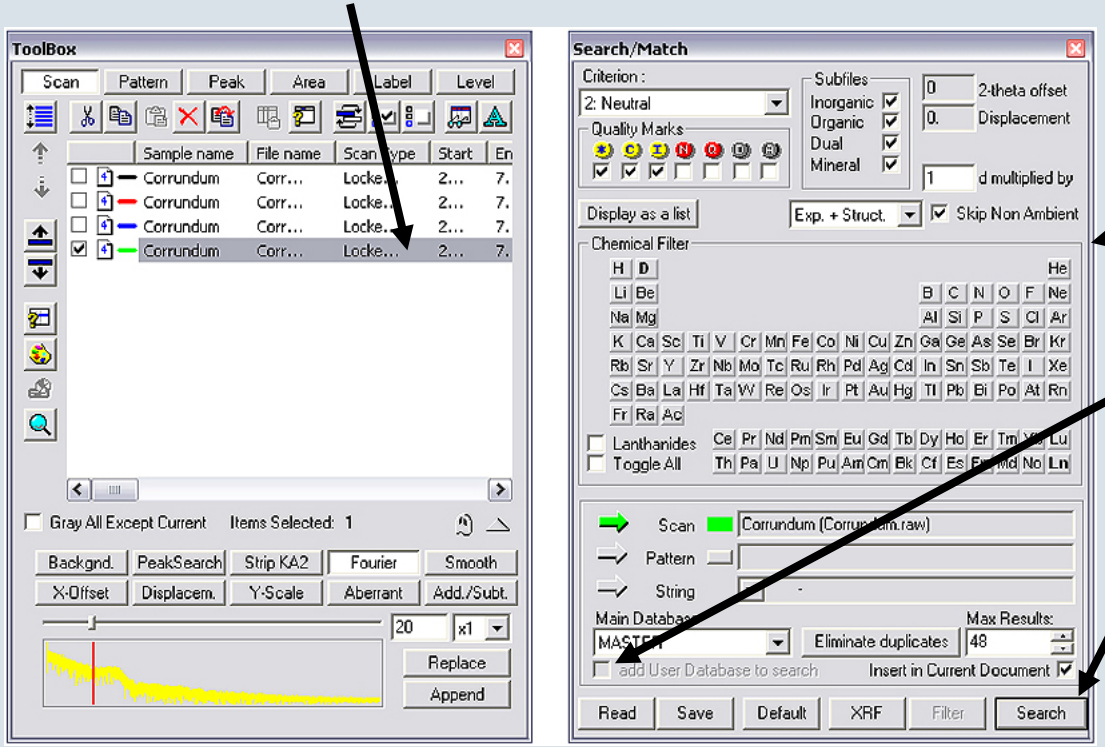
- Chemical Filter - Click the element to change its color
  - Red = not present
  - Grey = might be present
  - Green = must be present
  - Toggle all will change all of the elements' colors
- Scan
  - The scan which will be searched
- Eliminate Duplicates
  - If 2 patterns had the exact same name and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



Performing a Search/ Match

Bruker AXS

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

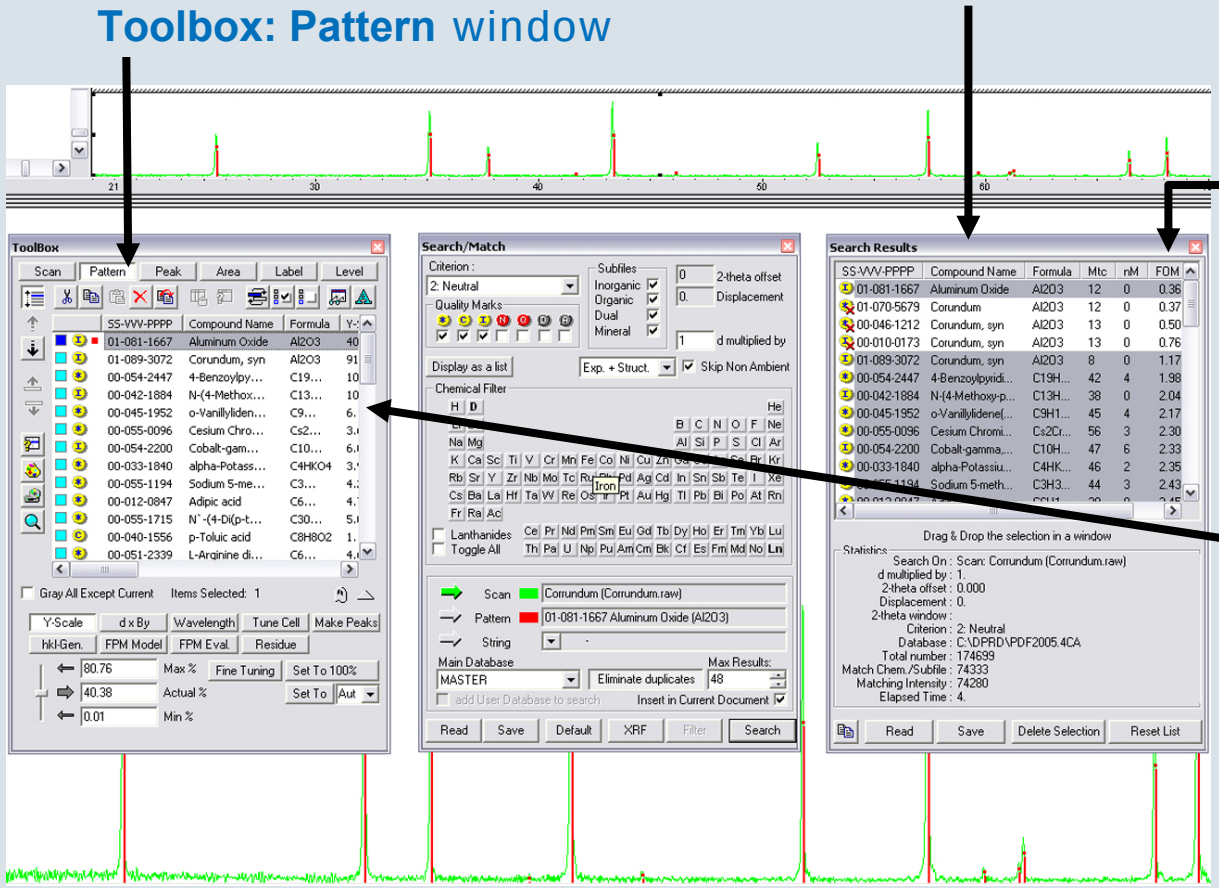


2. Input the appropriate settings
3. If a user database is present, check this box
4. Select **Search**

Search / Match Results

Bruker AXS

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

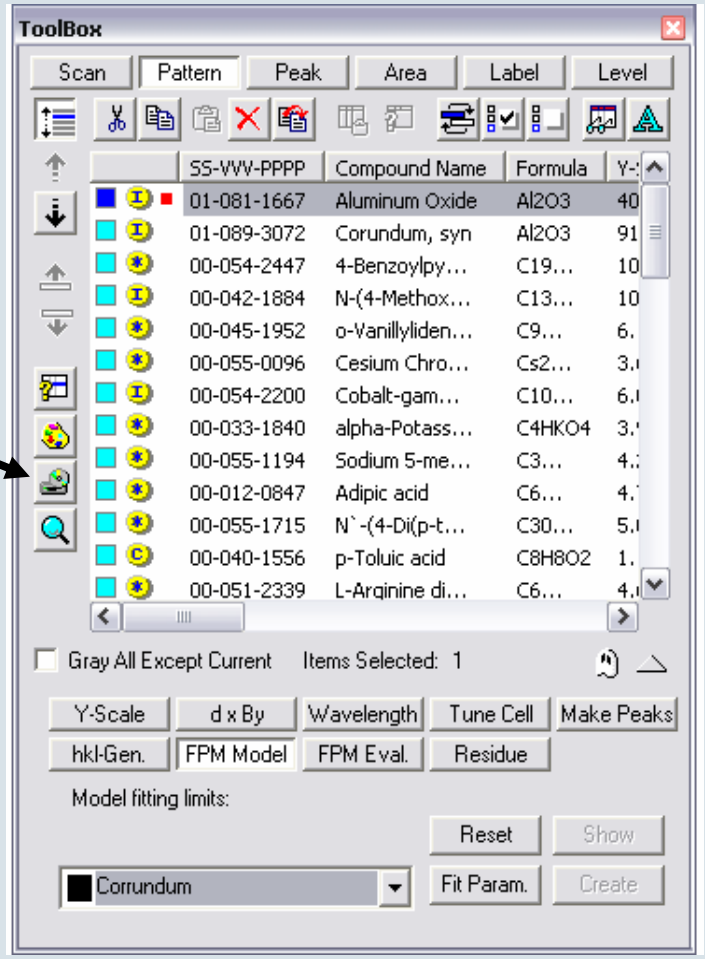


- The **Figure of Merit** (FOM) column gives a rough idea of how well the pattern matches. The lower the number, the better the match
- Highlighting a pattern shows the lines in the scan window

Displaying the PDF for a Pattern

Bruker AXS

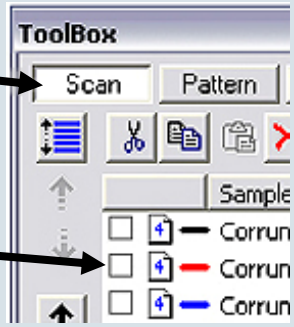
- Select the **PDF Database** button to view the PDF



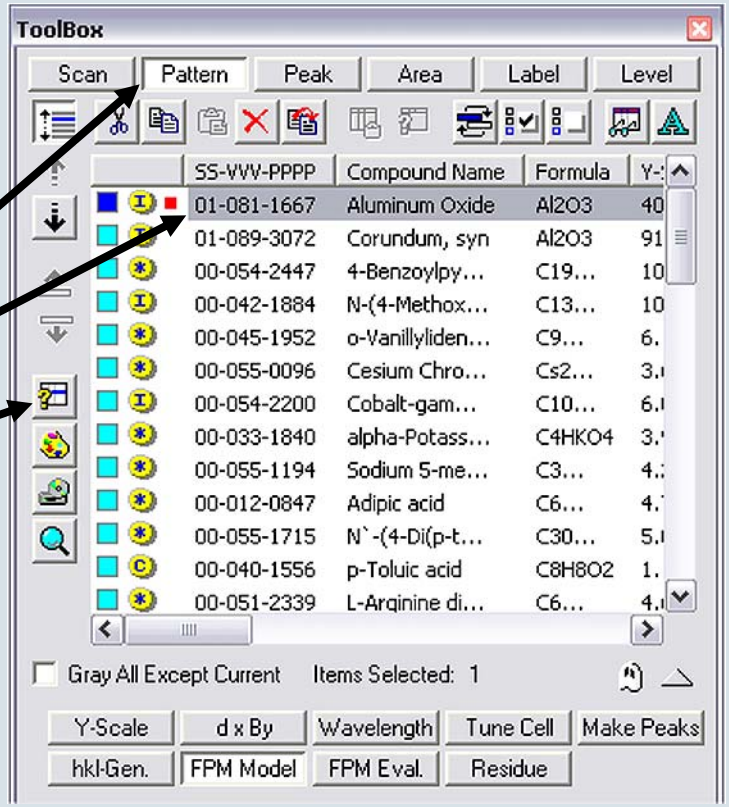
Refining Lattice Parameters

Bruker AXS

1. Navigate to the **Toolbox: Scan** window
2. Check the box next to the original scan so it is not hidden



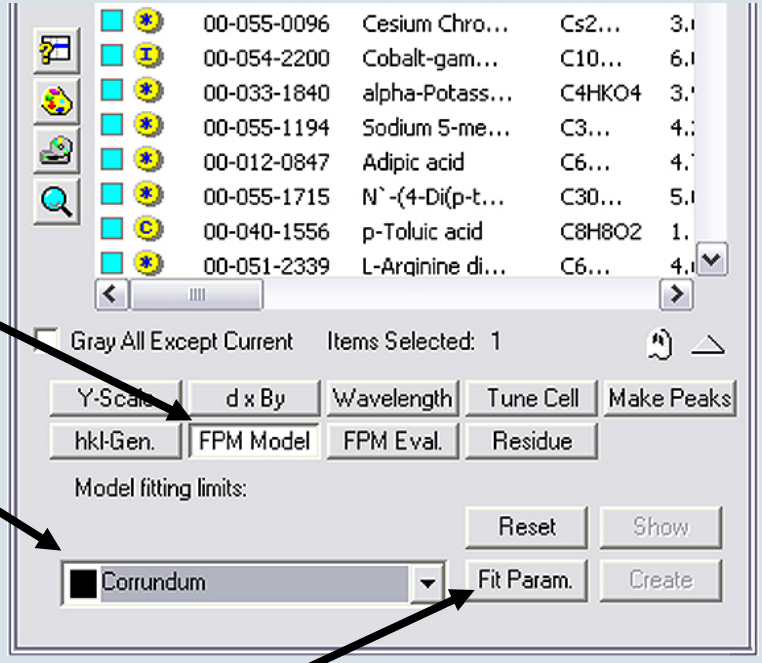
3. Return to the **Toolbox: Pattern** window
4. Highlight the pattern that fits the scan the best
5. Select the **Properties** button and check the **FPM boxes**



Lattice Parameter Refinement
(continued)

Bruker AXS

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

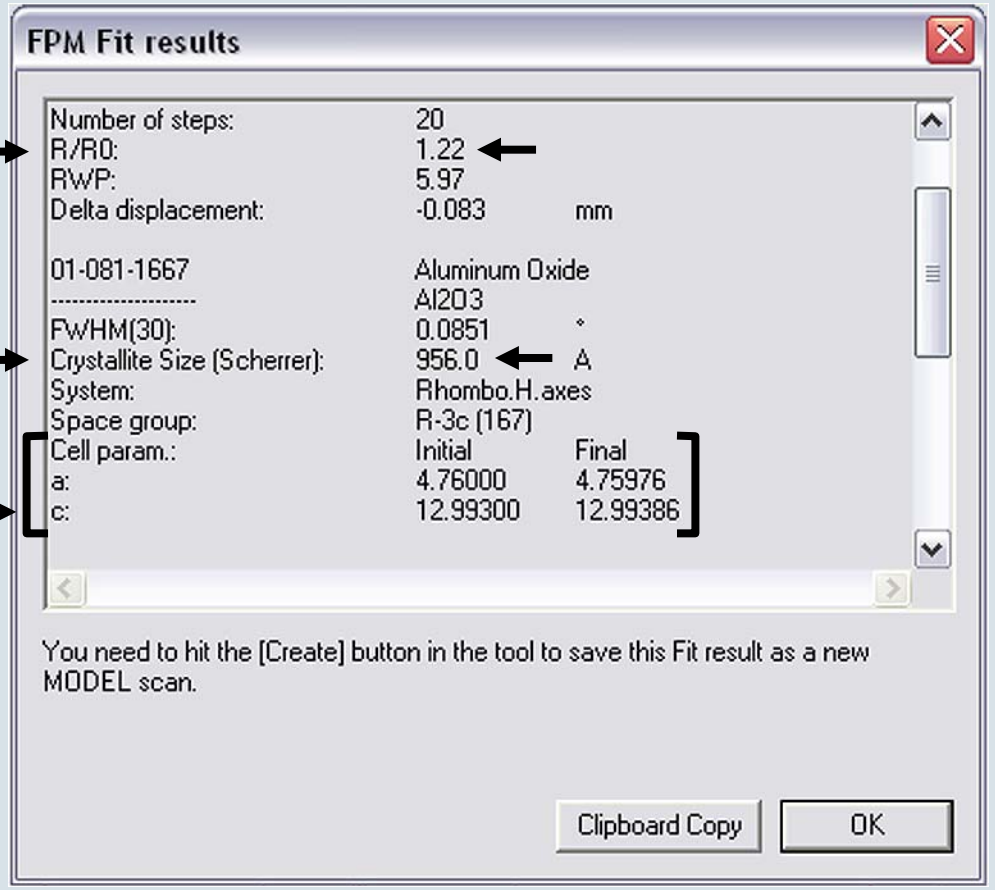


8. Select **Fit Param,** and the **Model Parameters** dialog will pop-up
9. In **Model Parameters** make sure none of the **Fixed** boxes are checked and select **OK**

Lattice Parameter Refinement Result

Bruker AXS

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



Bruker AXS