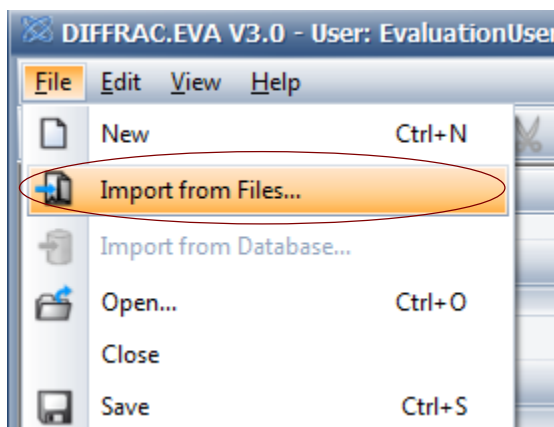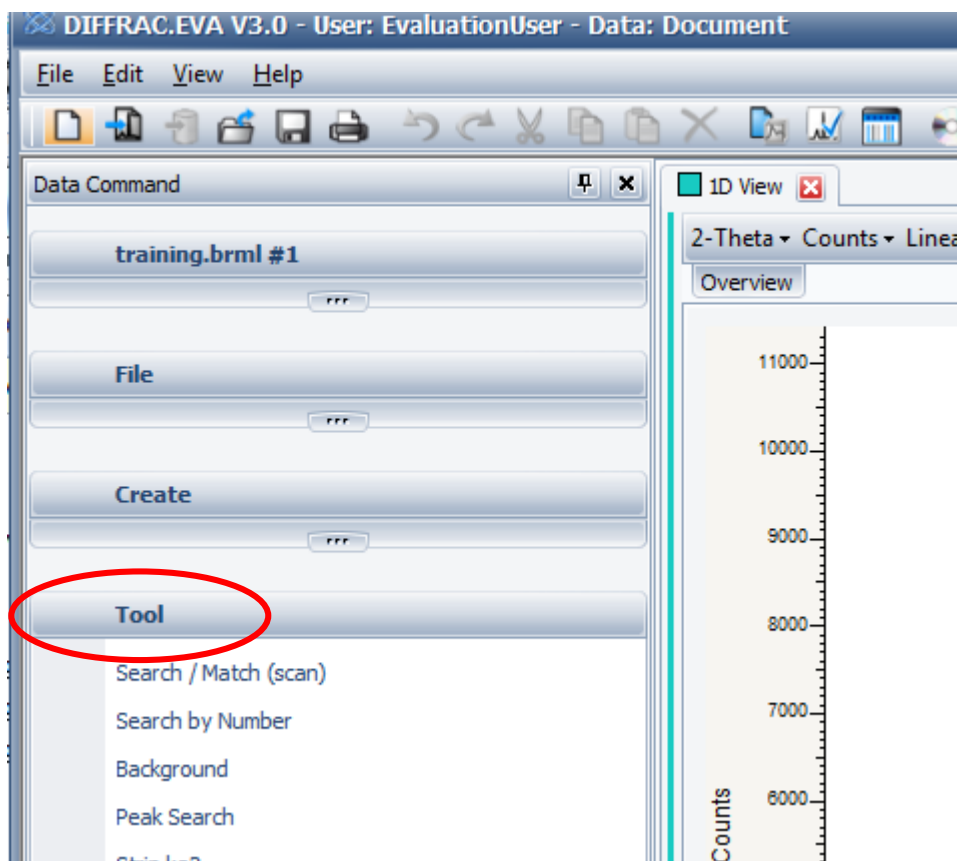# Notes on Work-Up of Powder Diffraction Data in EVA

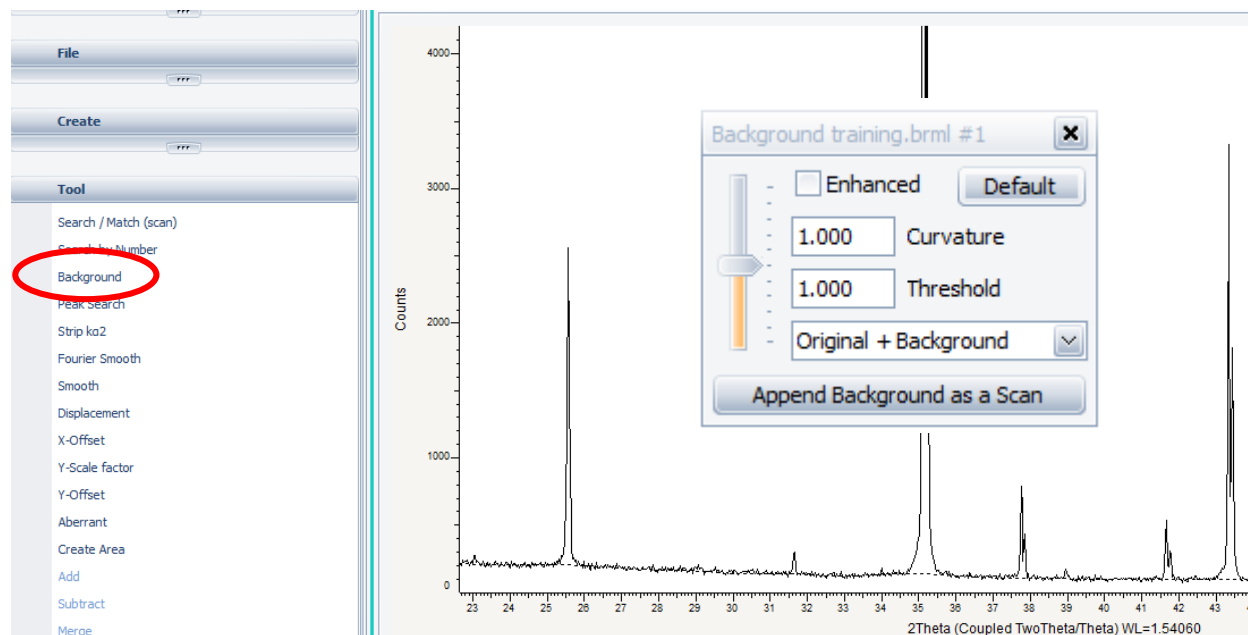The document is based on Yuliya Preger's notes.

Open EVA and import the scan. It should be present as a brml file.

Upon importing the scan, open the data command panel on the left and expand the 'Tool' section.

First, the background must be subtracted. Zoom in at a low angle part of the pattern by drawing a rectangle and click Background in the Tool menu.


The background is approximated by the dashed line. Adjust the vertical slider to get the best fit. Open the dropdown menu and select 'background subtracted.' Close the dialog box.

Next, subtract the Kα_2 peaks. Zoom out on the pattern by depressing the left mouse button and dragging the cursor to the left. Zoom in at higher 2theta values. Go to the 'Tool' menu and select 'Strip Kα_2.'
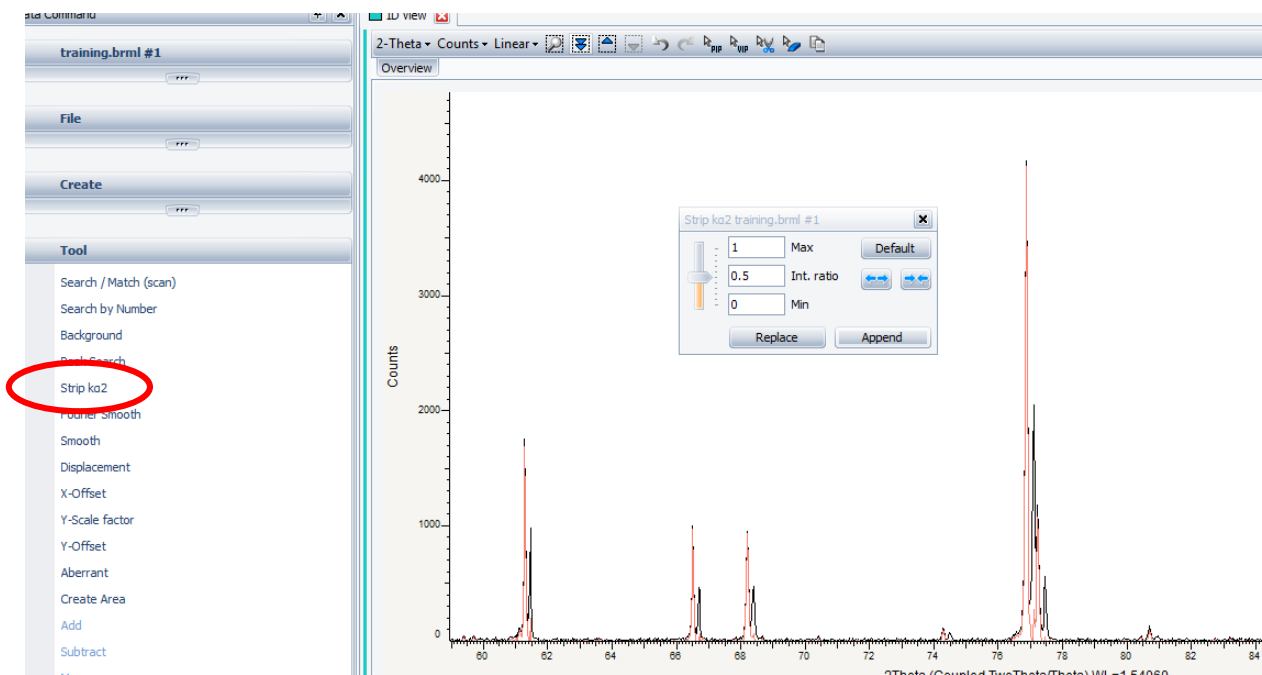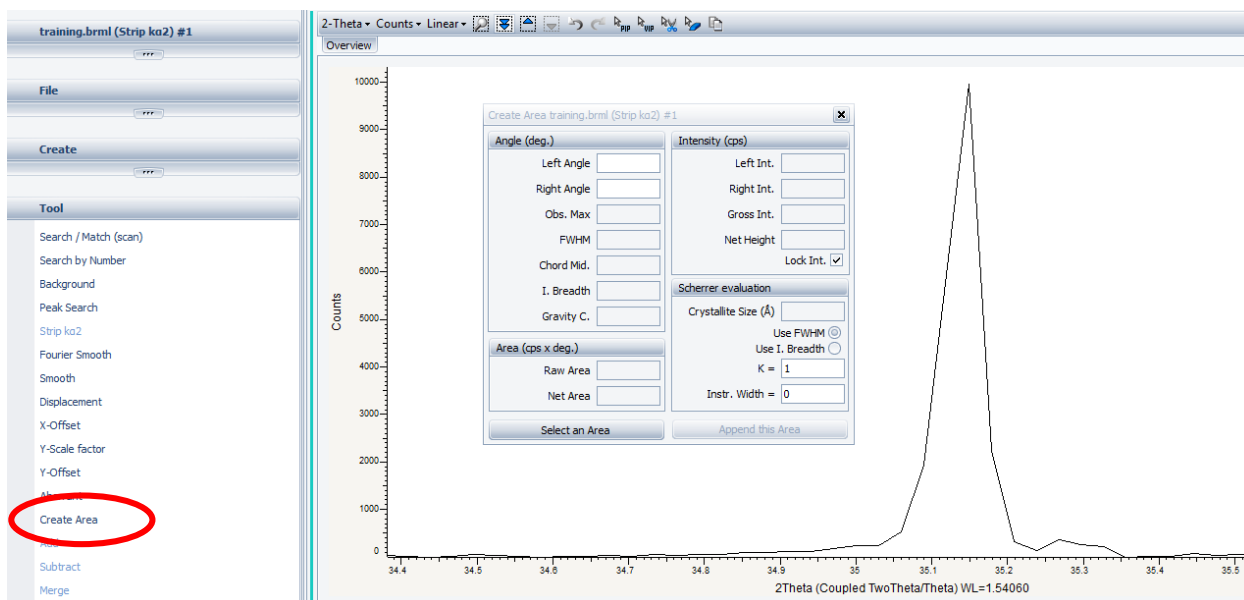
Adjust the slider to get the best fit and select 'Replace'. Use 'Append' if you wish to save the original pattern for later. The modified pattern should then look like:
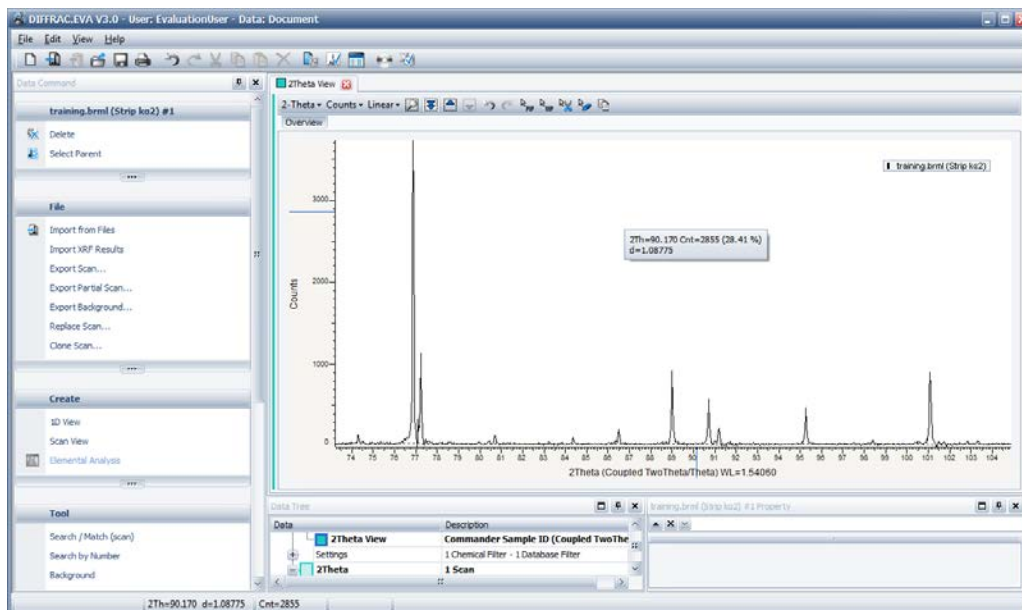

Next, if working with a known sample, determine whether the reference peaks are positioned at the correct 2 theta values. For corundum zero in on the highest peak at 35.149°.

Select 'Create Area' in the tool menu.

Click on 'select an area' in the bottom left corner of the menu that pops up. Roll the tool that appeared over the area of interest (e.g. from the low angle background of your peak to the high angle background).
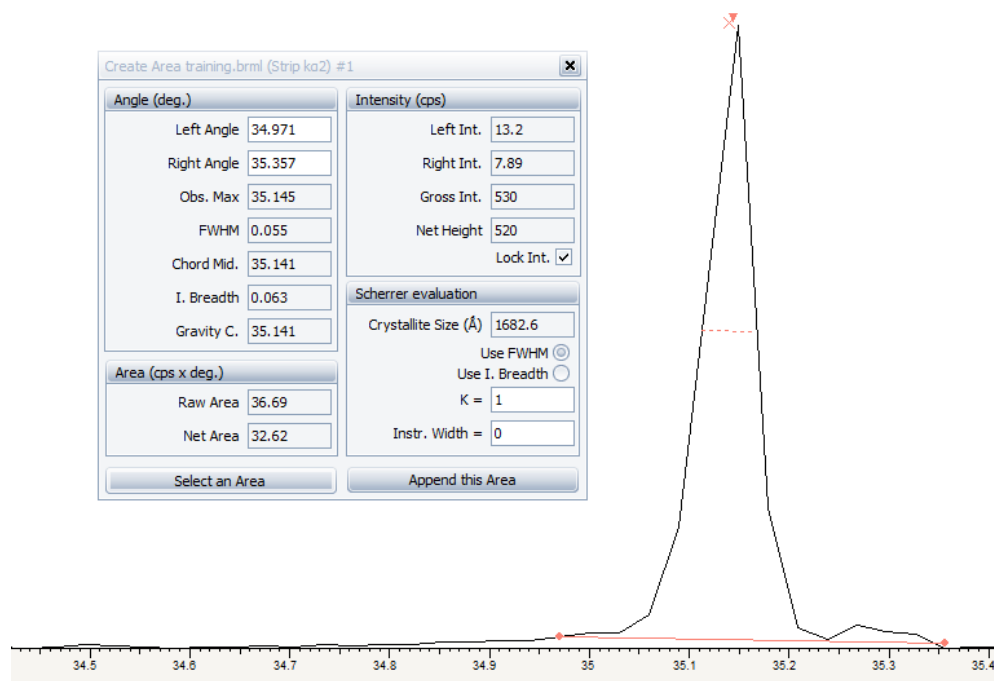

From the box on the left, the Observed max is 35.145. The literature value for this sample is 35.149. The instrument precision is 0.01 degree. The difference between 35.145 and 35.149 is less than 0.01, thus no shifting of the pattern is necessary.

However, if the observed maximum is too far from the known value, select 'Displacement' in the left hand 'Tool' menu and adjust the slider to shift the pattern.
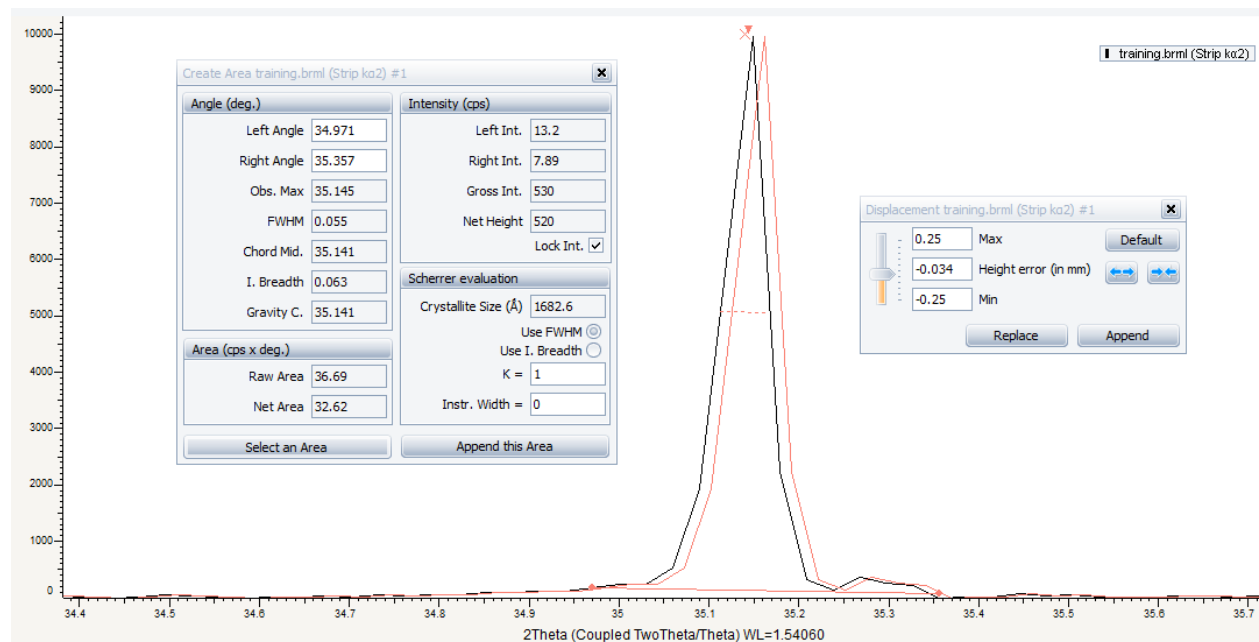
Next, identify the elemental composition of the sample. Select 'Search/Match (scan)' in the lefthand 'Tool' menu. In the window that pops up, select the 'Chemical Filter' tab.
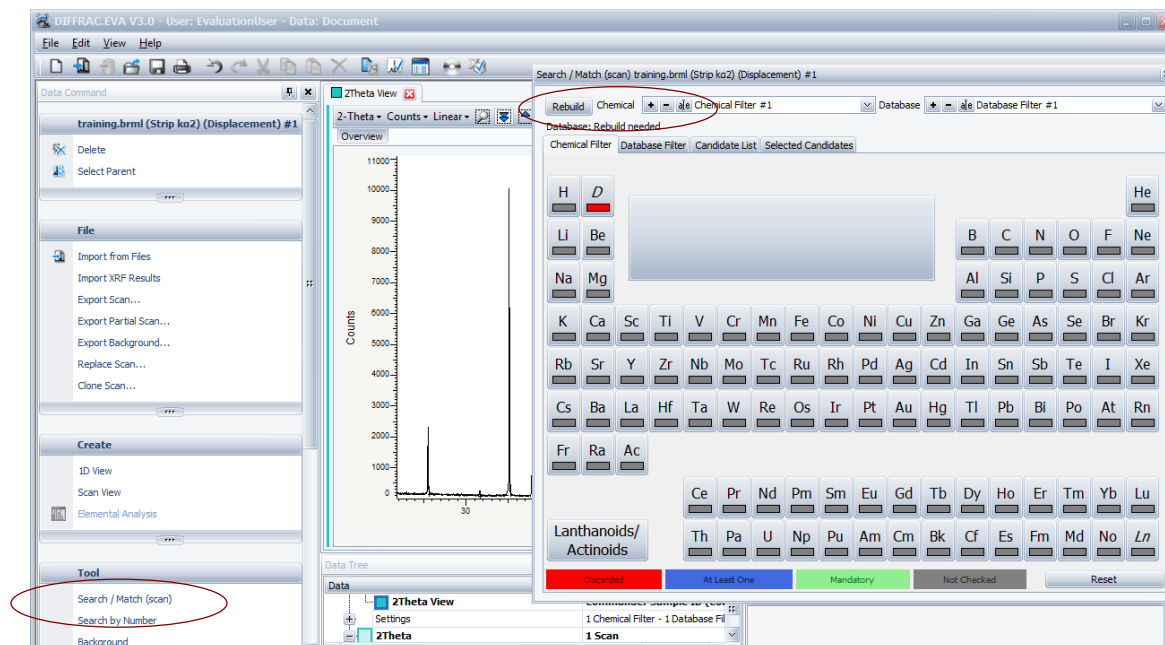
Right click an element to indicate whether it should be: discarded, included, or whether at least one of several elements under consideration must appear.
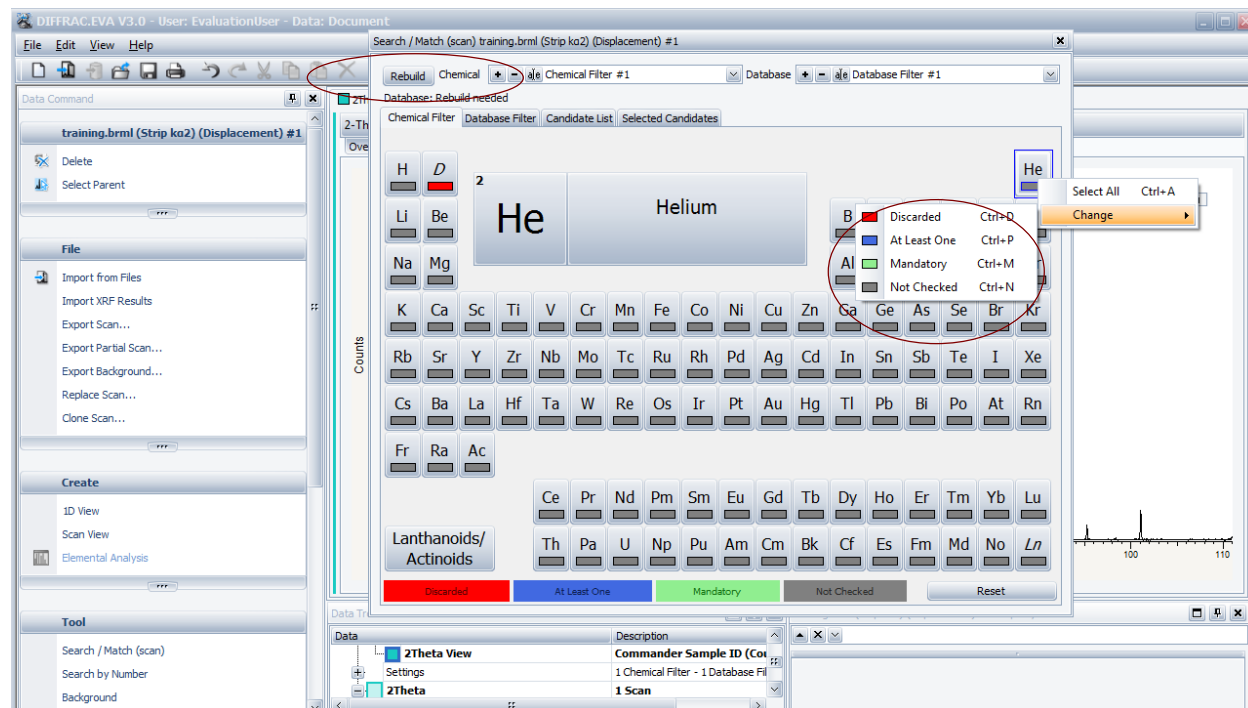
By left-clicking and dragging, blocks of elements can be highlighted at once. Upon assigning the appropriate logic to selected elements, click 'Rebuild' in the upper left hand corner to apply the filter.

Go to the 'Candidate List' tab.

In the bottom right corner select the type of the pattern (simple/neural/complex) and press the Match button. A list of possible matches is displayed. The entries are sorted by figure of merit.

Additional modifications that can be made to the pattern include inserting a picture and adjusting the peak height.

To insert a picture, click 'PIP' in the upper toolbar. Highlight a small peak, then click anywhere on the pattern to generate the new picture.

To adjust the height of a small peak, click 'VIP' (near PIP). Highlight a small peak. Adjust the sliding bar on the image to magnify the peak as desired.