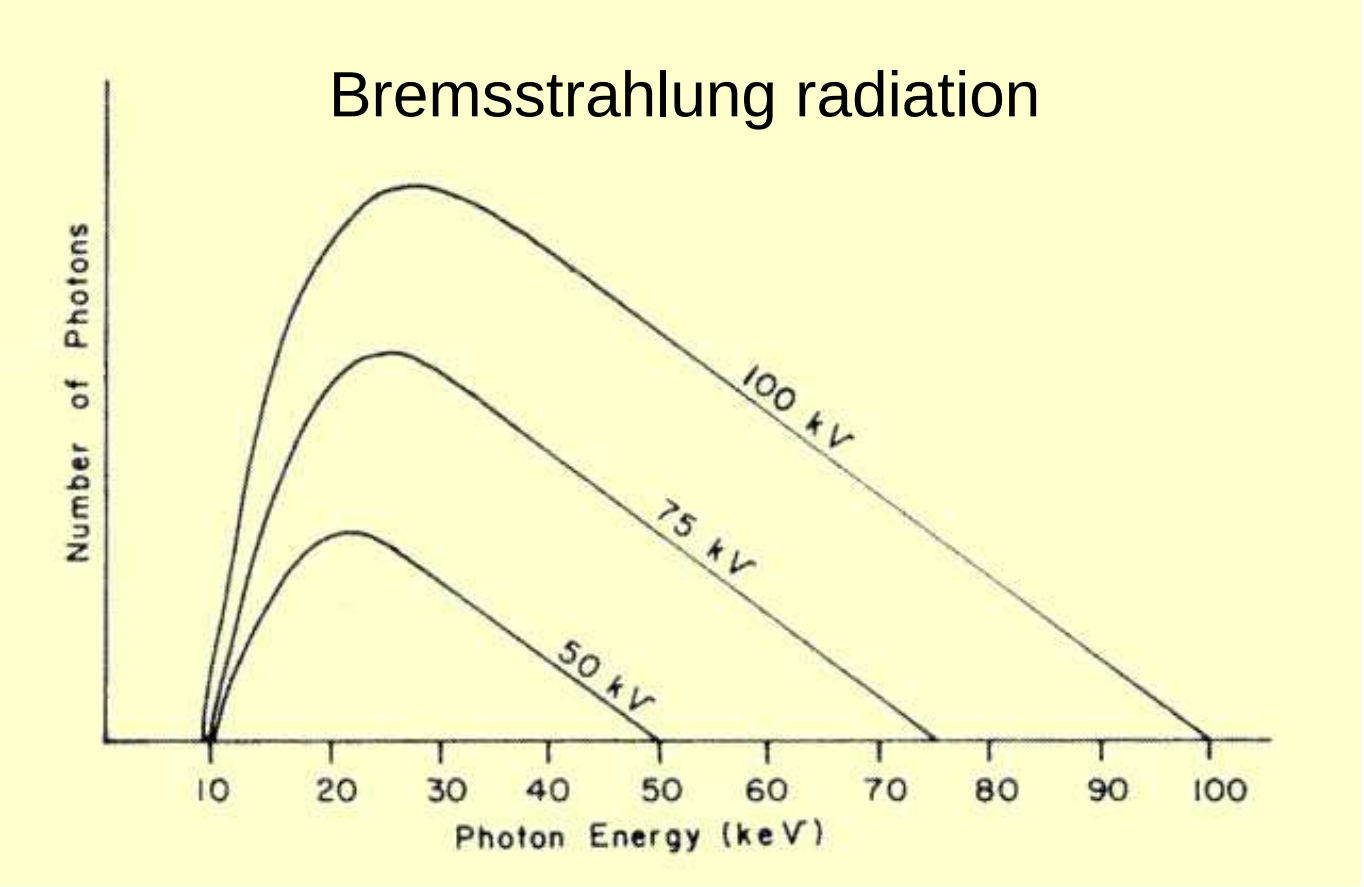
Qualitative analysis tutorial for Tracer III SD and V+ data

Outline

- What does the spectrum mean?
- What to watch out for
- How to normalize
- Using Artax

What does the spectrum mean?



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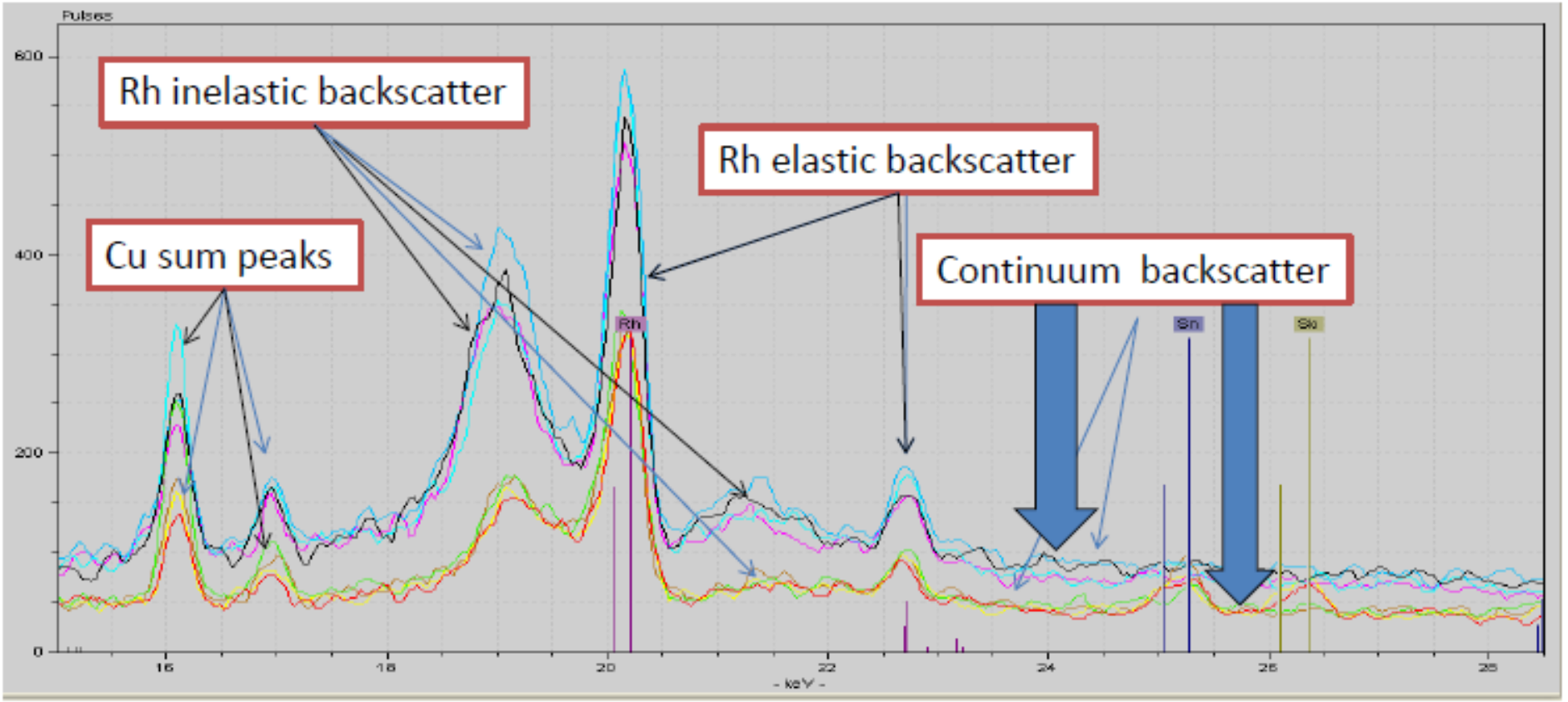

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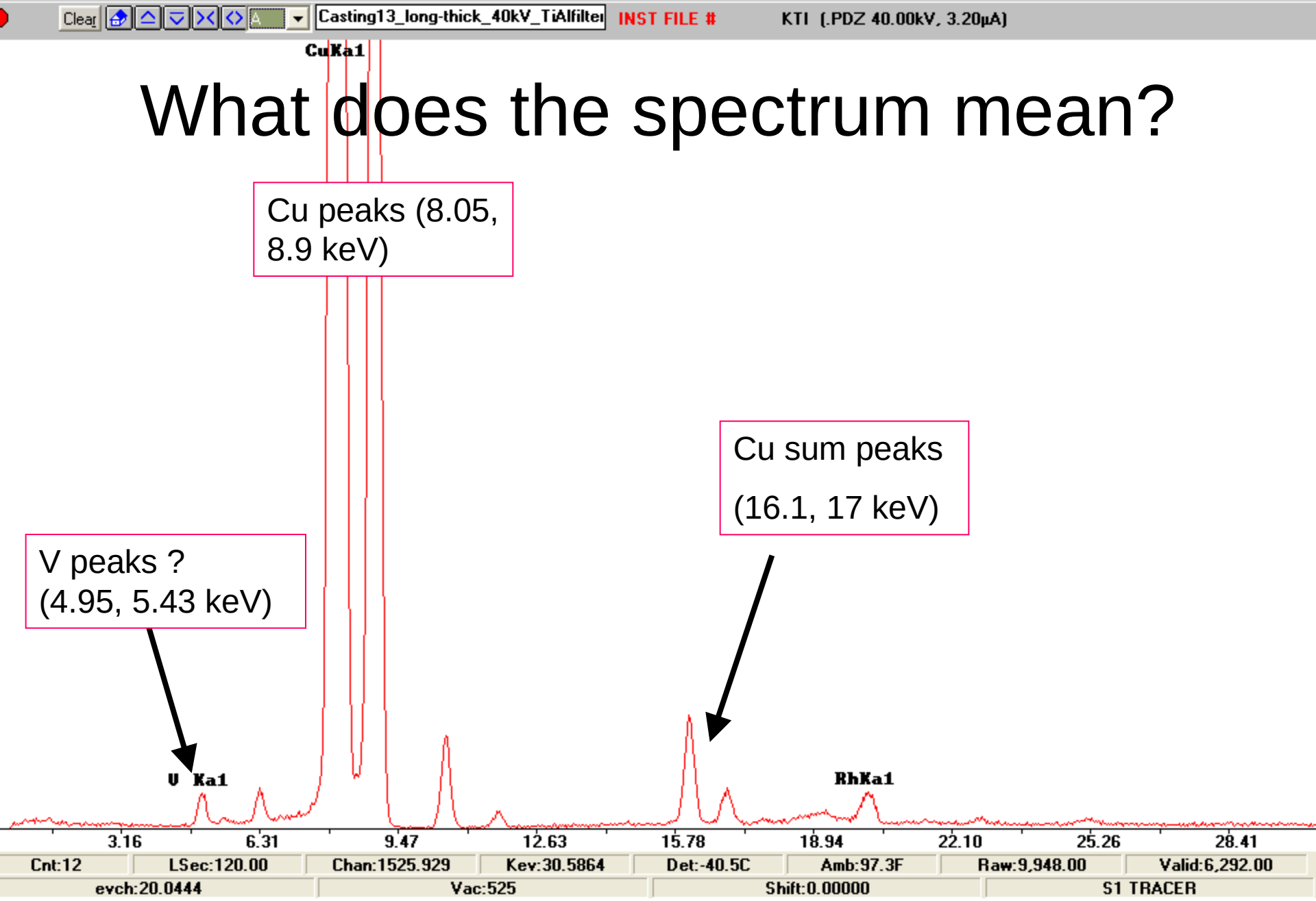
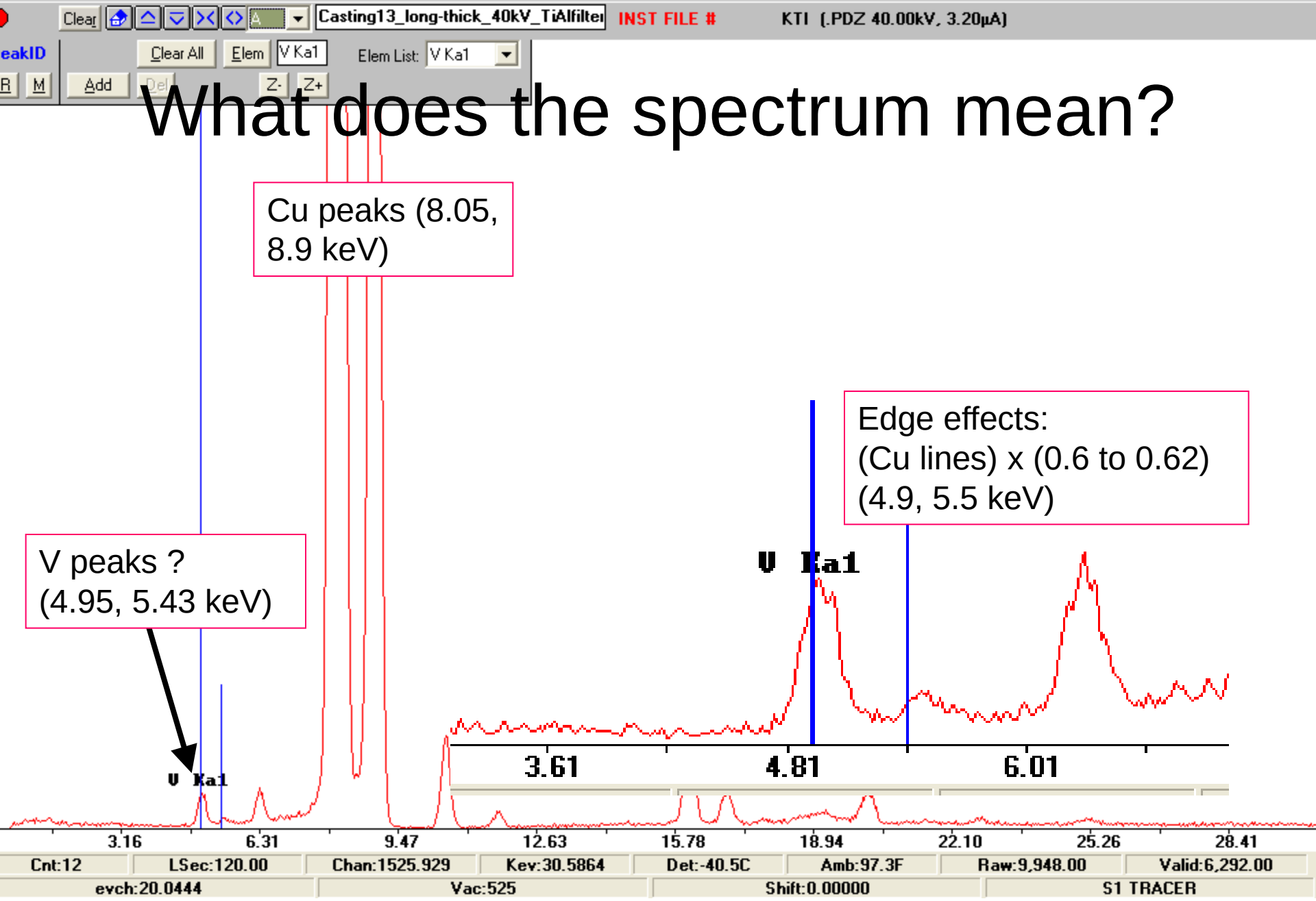


Copper alloy

What does the spectrum mean?



Copper alloy

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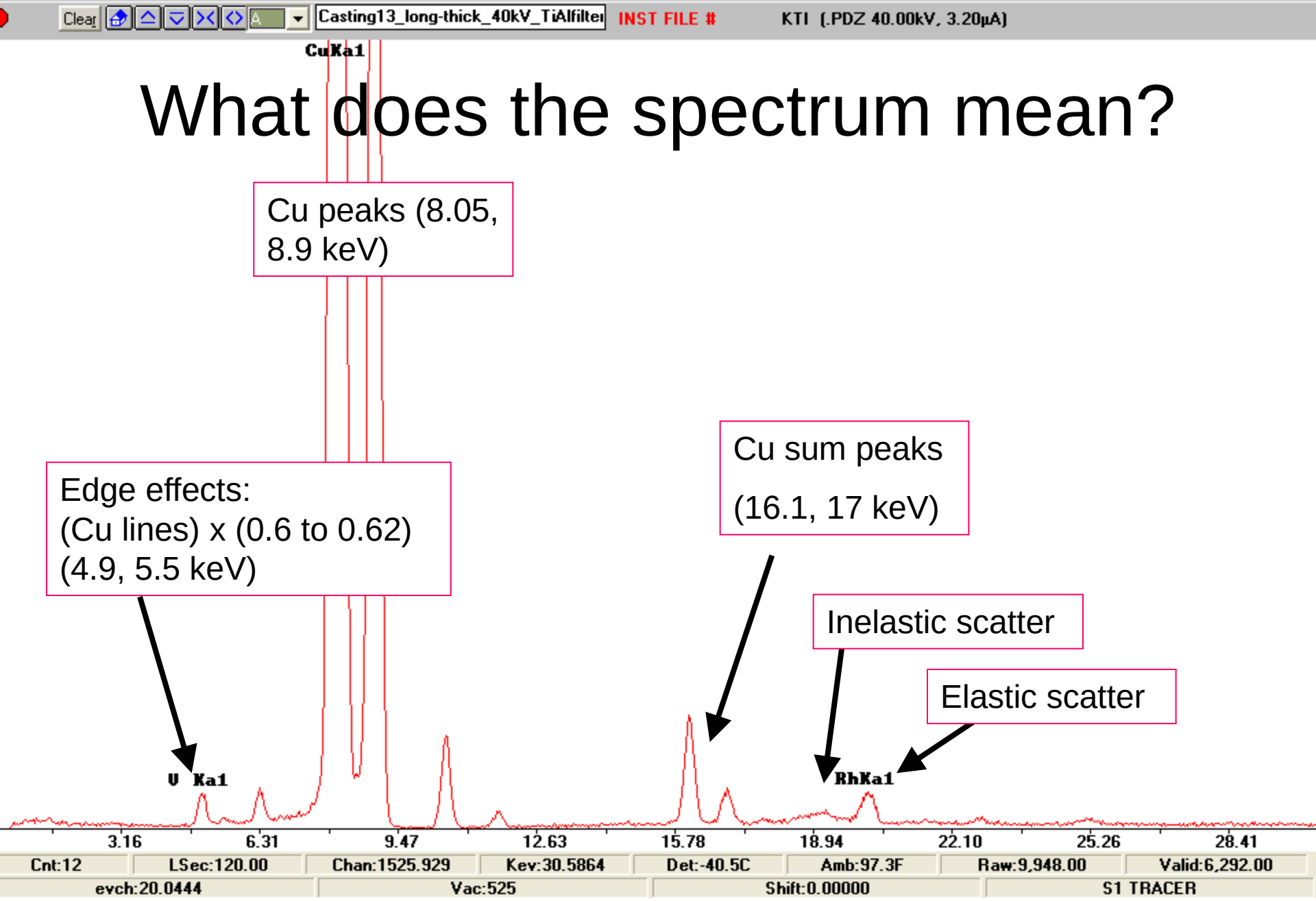
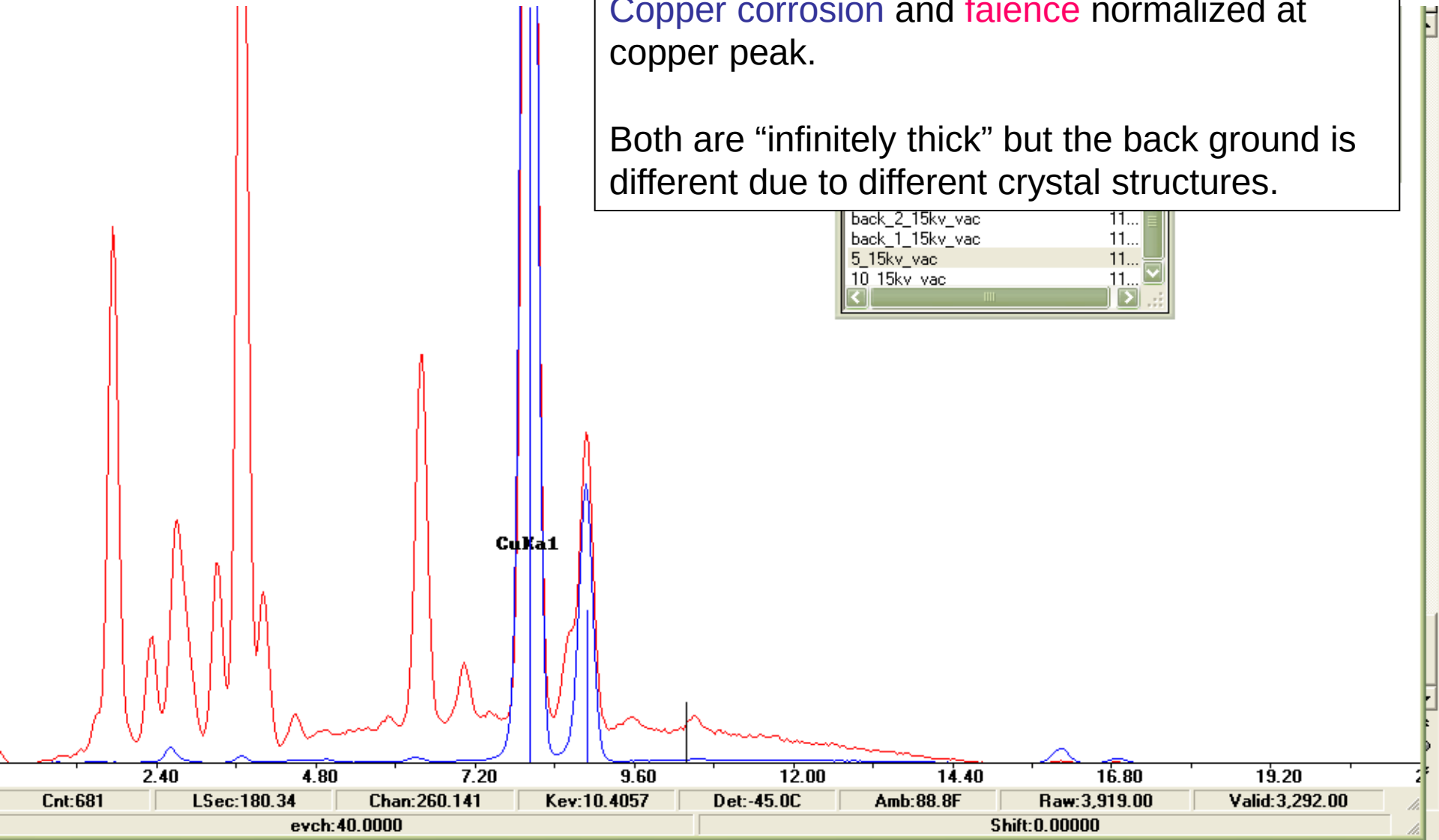


Copper alloy

What does the spectrum mean?

Copper corrosion and faience normalized at copper peak.

Both are “infinitely thick” but the back ground is different due to different crystal structures.



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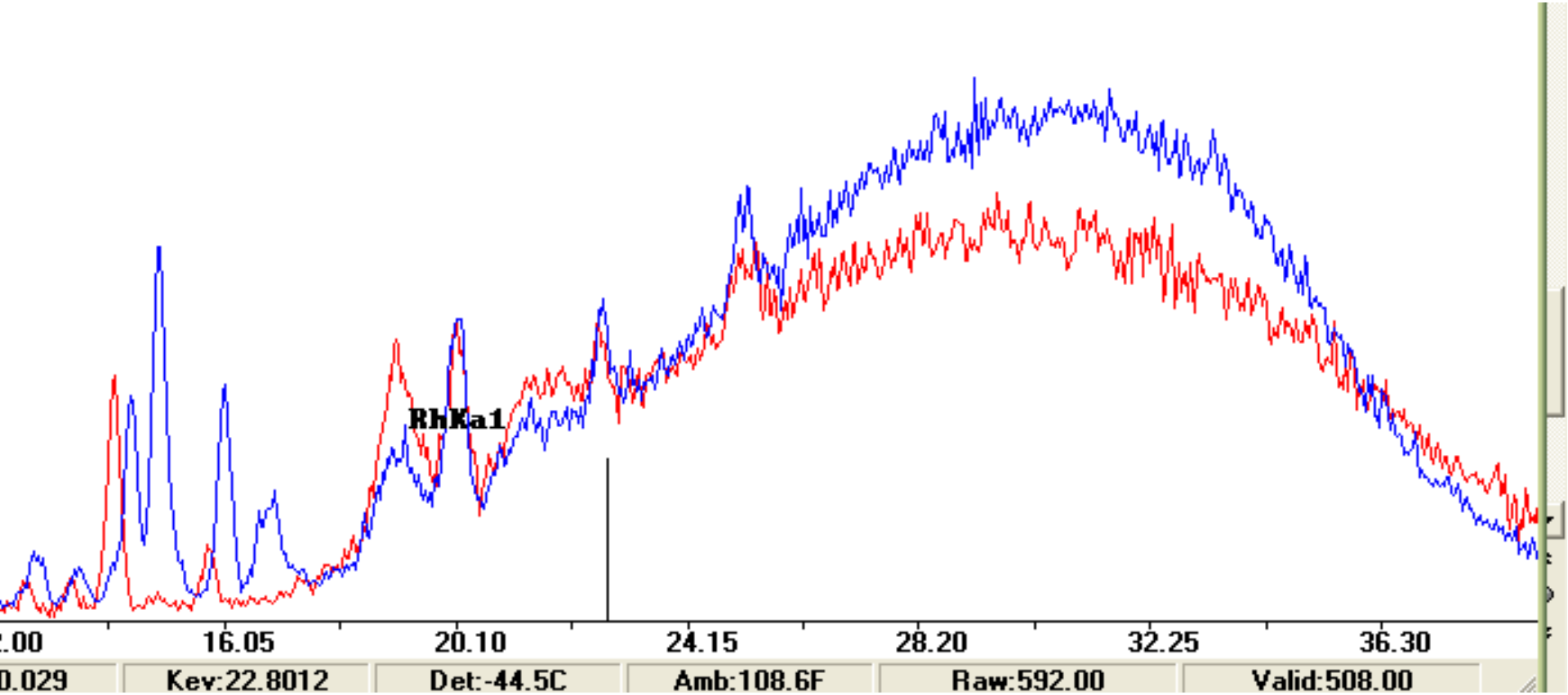


Copper ore (XL) faience (glass) with same filters and beam settings
Normalized at Rh (note: elastic vs inelastic peaks)

What to watch out for

- Matrix effects
- Inhomogeneous materials
- Sample size (small or thin samples have larger background)
  - Choose “infinitely thick” samples

How to get around these… normalizing

- Normalize to:
  - Background
  - Major elements
- Element ratios
- Use filters
- Monitor counts
- Carefully select instrument settings
- Use same settings to compare spectra!!

Now open Artax and open your Spectra in Artax

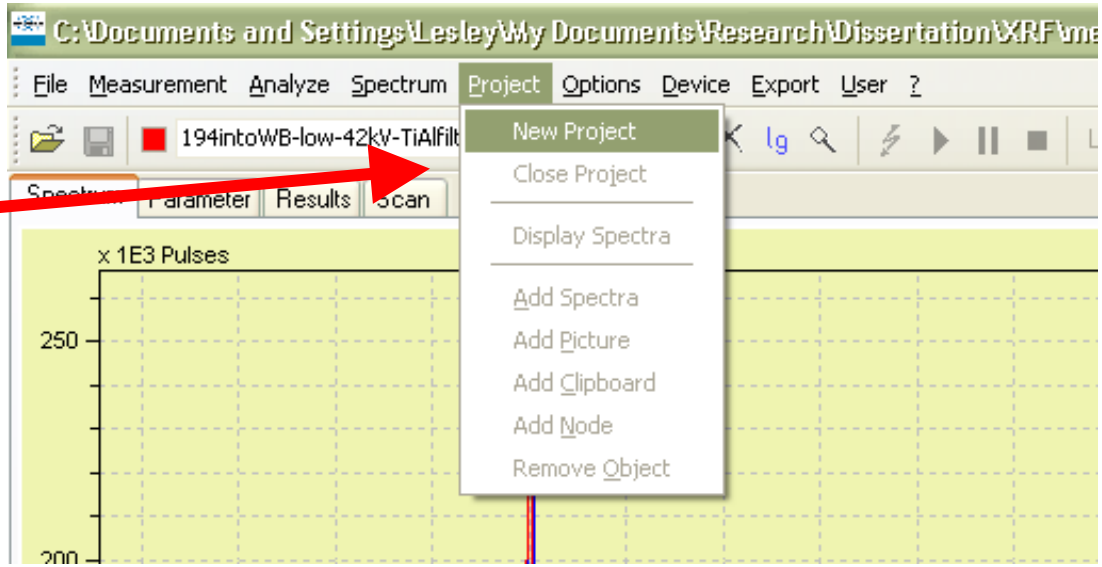
- Click on File and open spectra
- Make sure files of type is on txt
- you can only have 100 spectra on the display at any one time, but you can have up to 4000000 spectra in your Points folder that you do the analysis on.
- So open 100 spectra or less and then add them to the Points folder. Then clear all the spectra on the display and open the second set of 100 or less and click on add spectrum to add those 100 to the Points folder and then clear all the spectra on the display and open the next group and add them to the Points folder.
- Whatever is on the display can be added to the Points folder so you do this cycle until all your spectra are in the Points folder.
- Then you do your analysis on the Points folder.

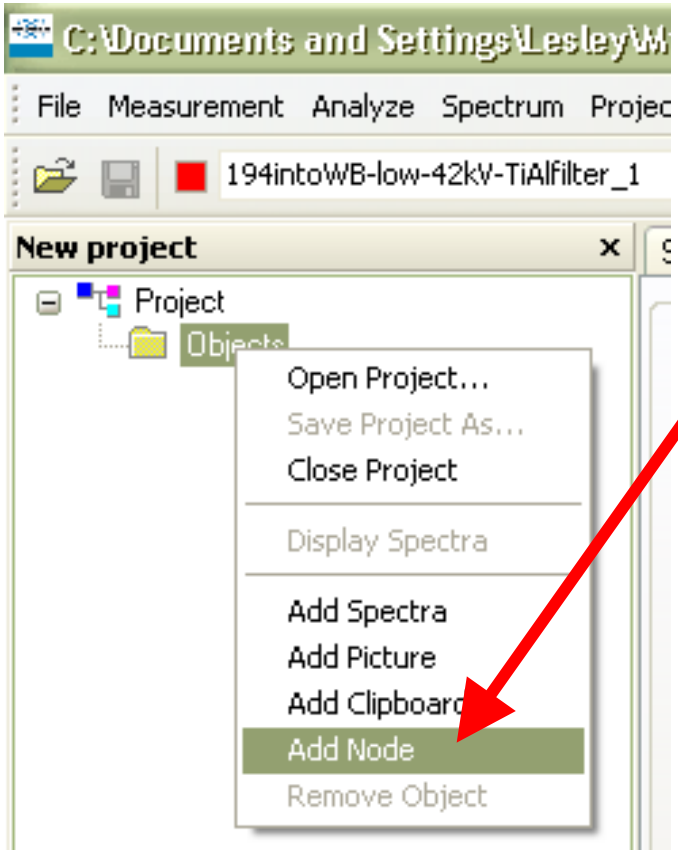
Using Artax for qualitative analysis

1. Read in your pdz files from the S1PXRF data up to 100 of them at a time
2. Open ARTAX and make a new project

Open all spectra of interest using Ctrl + O or File → open spectrum…

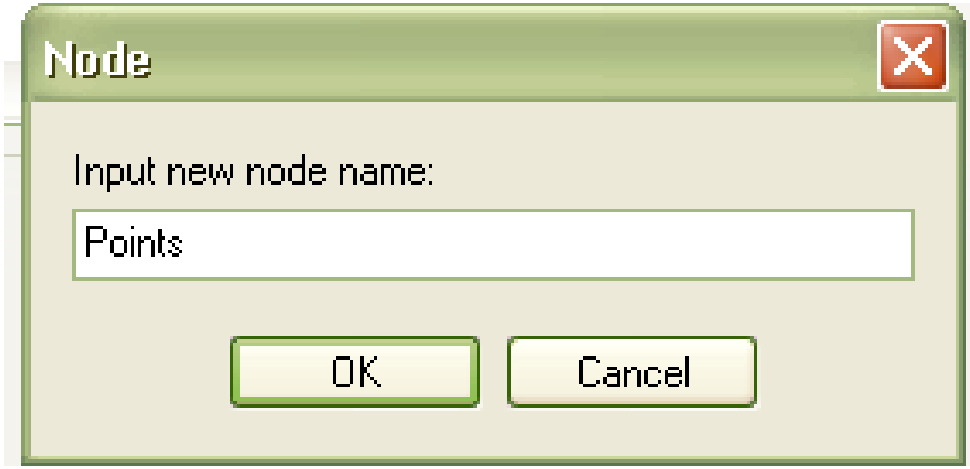
Then start a new project



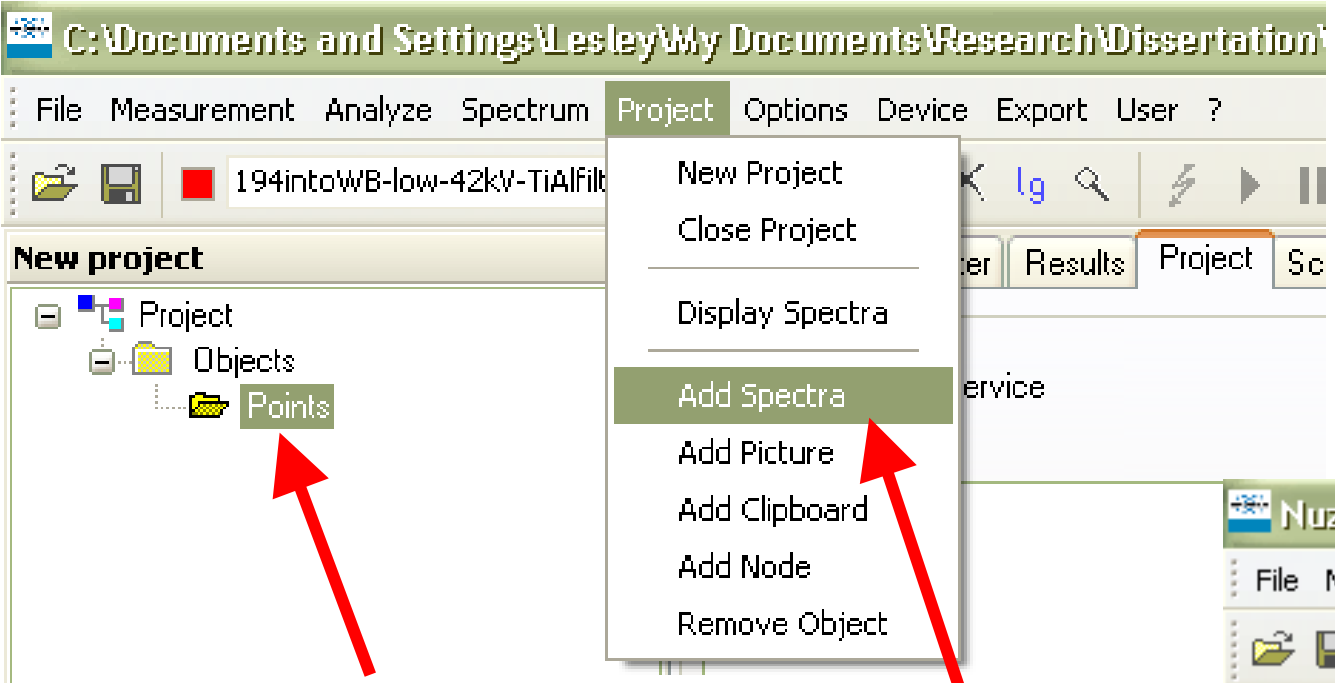


Right click on Objects in the project pane, select Add Node

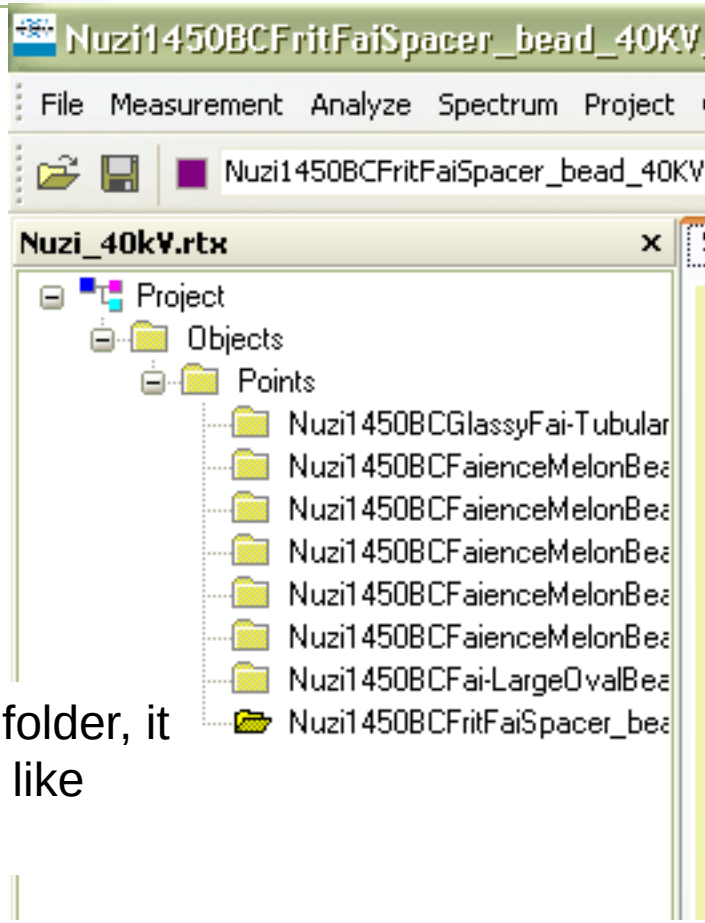
A new window will open



Name the node “Points” (with capitol P)



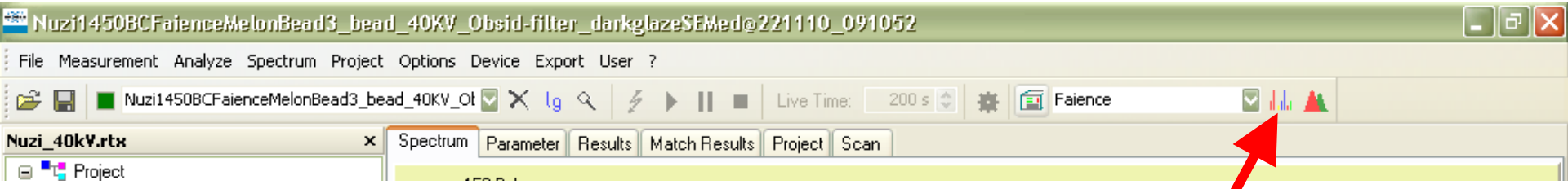
Click on Points folder. Go to Projects and select Add Spectra.
All of the opened spectra will be added to this node



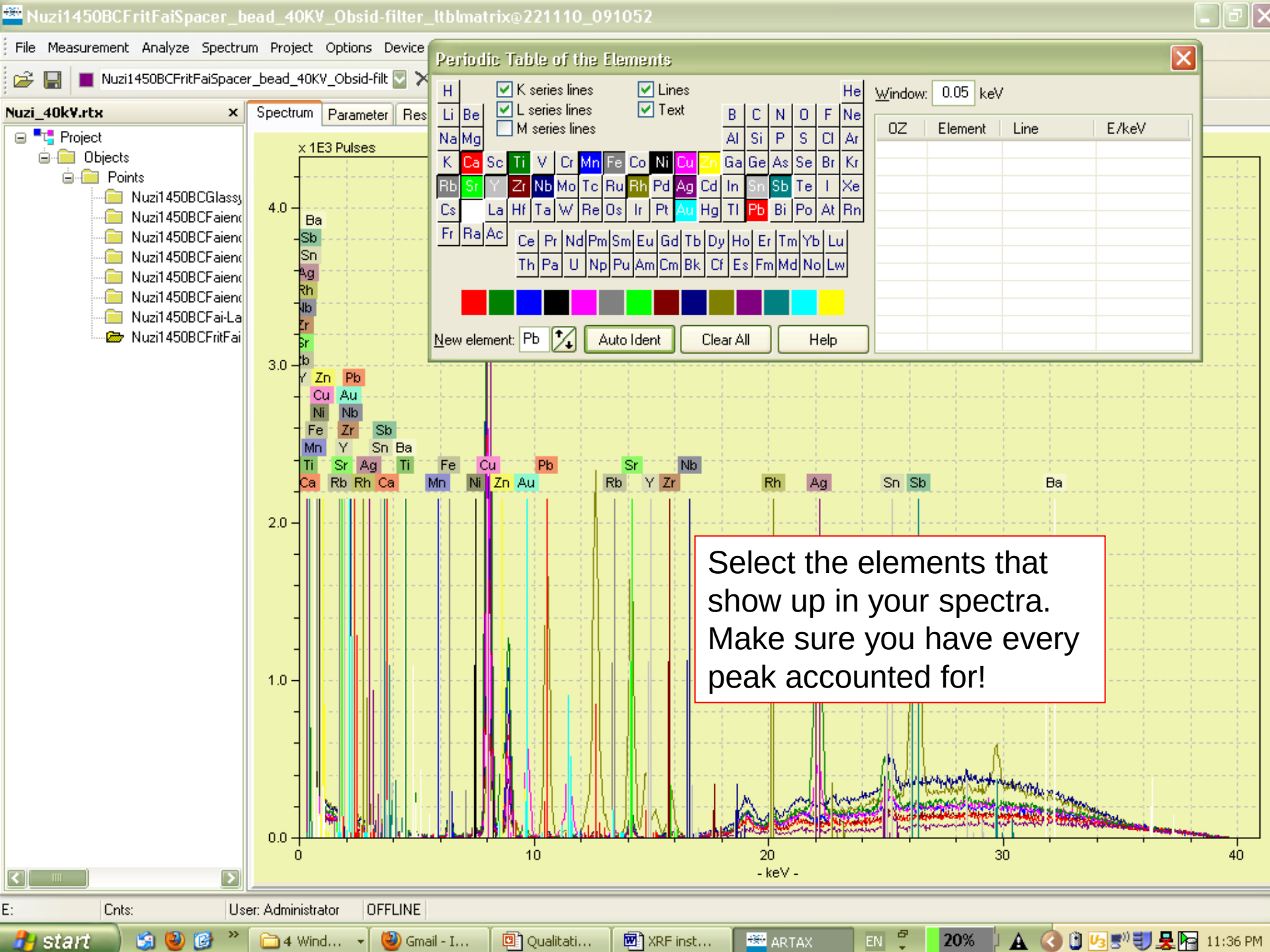
When you expand the folder, it should look something like this.

Using Artax for qualitative analysis

1. Create txt files in S1PXRF
2. Open ARTAX and make a new project
3. Choose elements



Select this icon to open the periodic table of elements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Nuzi1450BCFaienc
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Ba
Select the elements that show up in your spectra. Make sure you have every peak accounted for!
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Cnts:
User: Administrator
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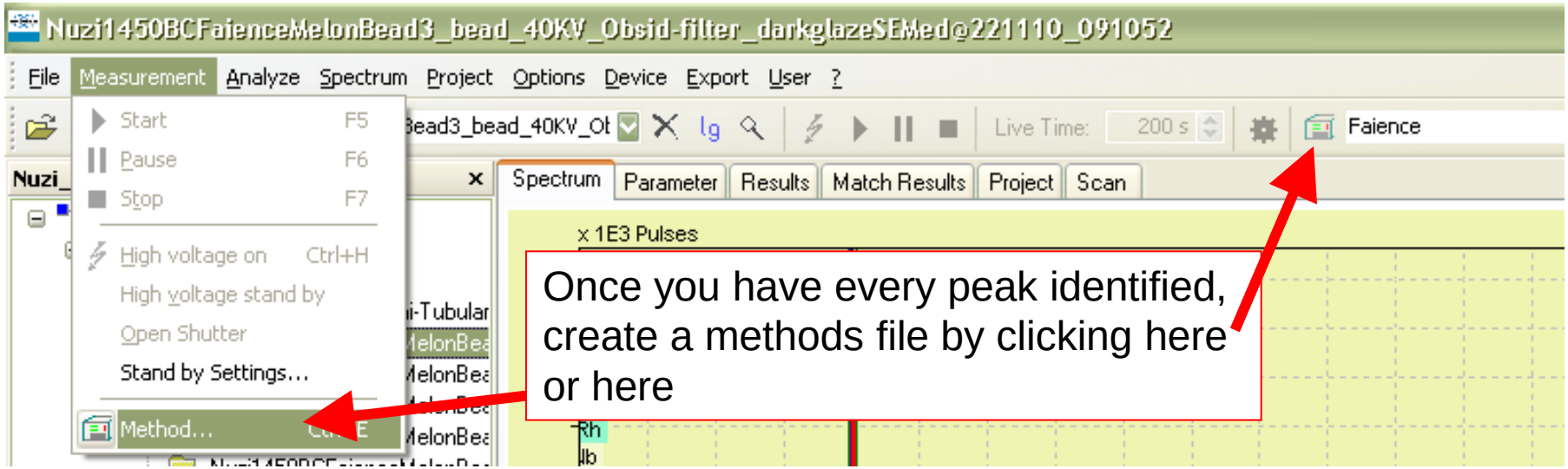
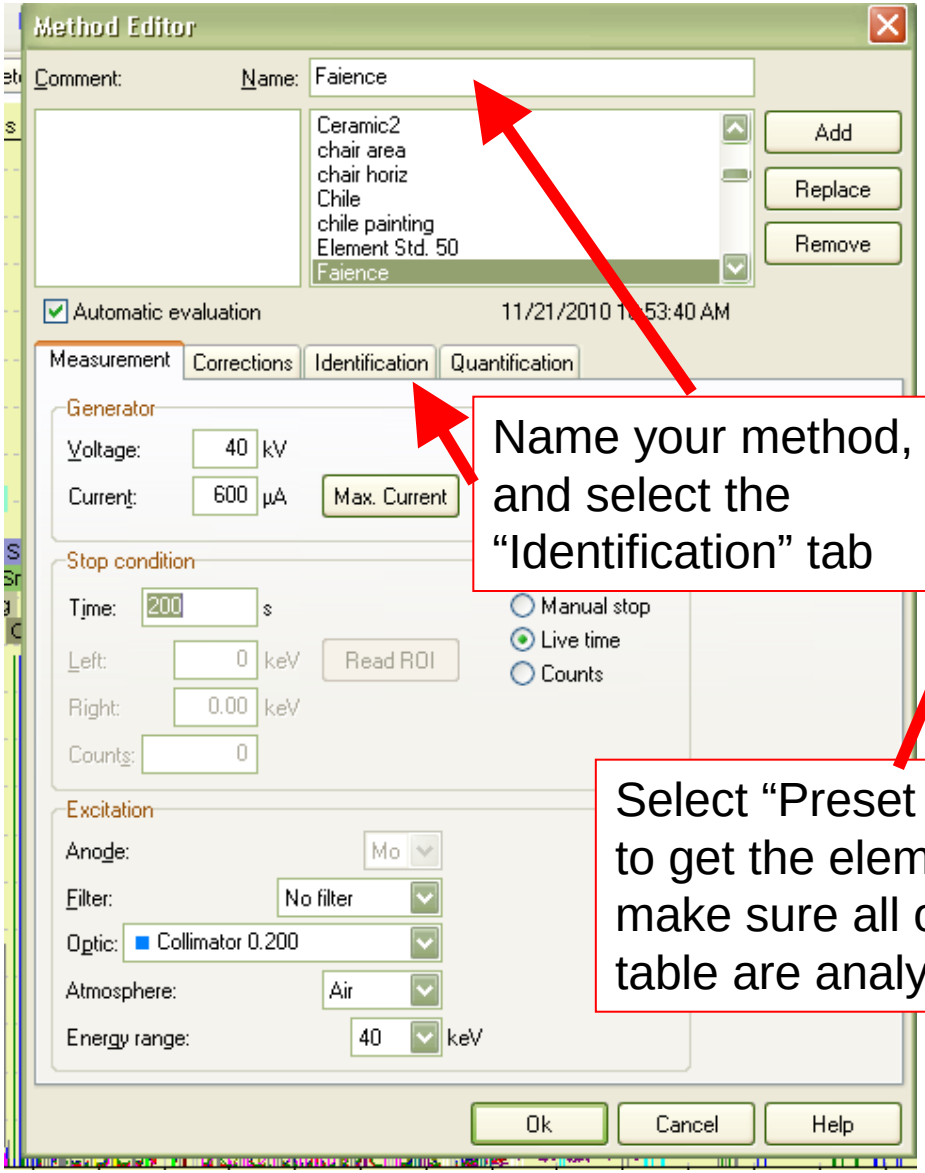
Using Artax for qualitative analysis

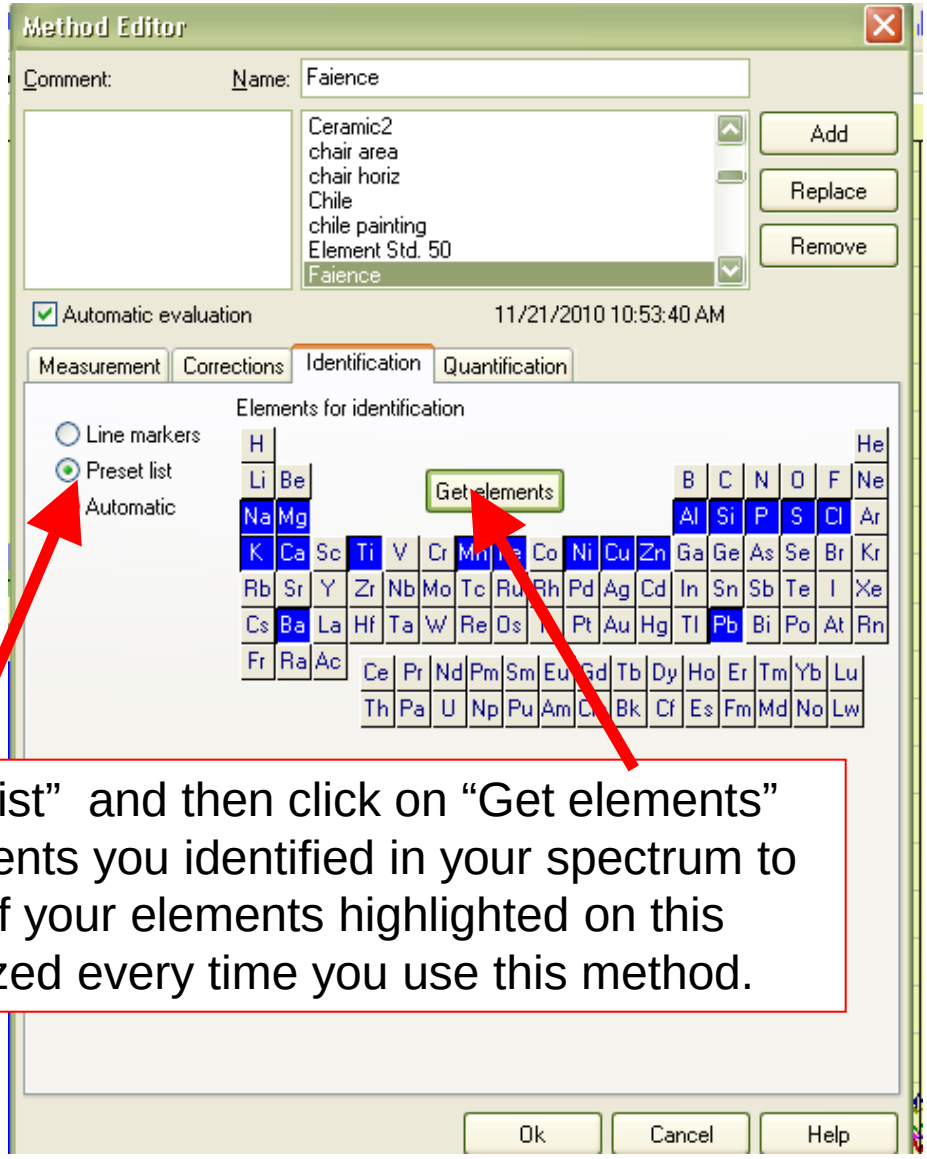
1. Create txt files in S1PXRF
2. Open ARTAX and make a new project
3. Choose elements
4. Create Methods file



A new window will open

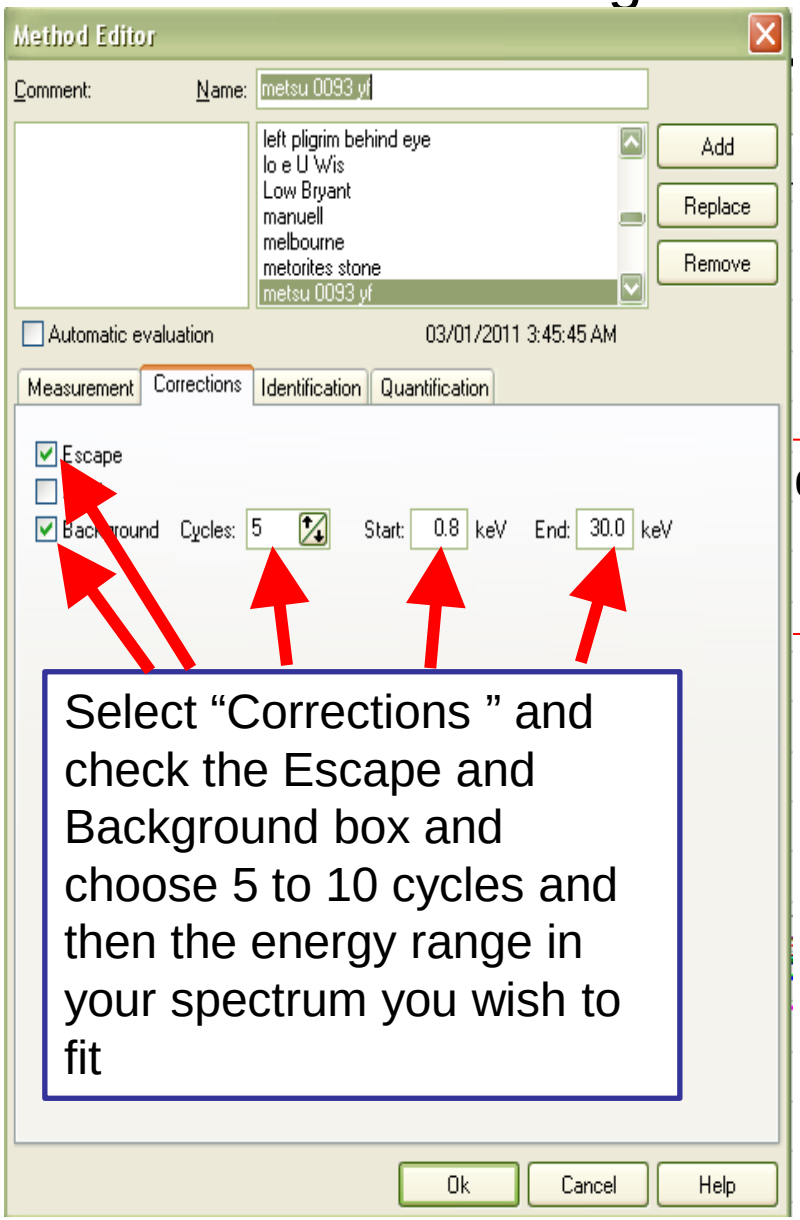


Name your method, and select the “Identification” tab

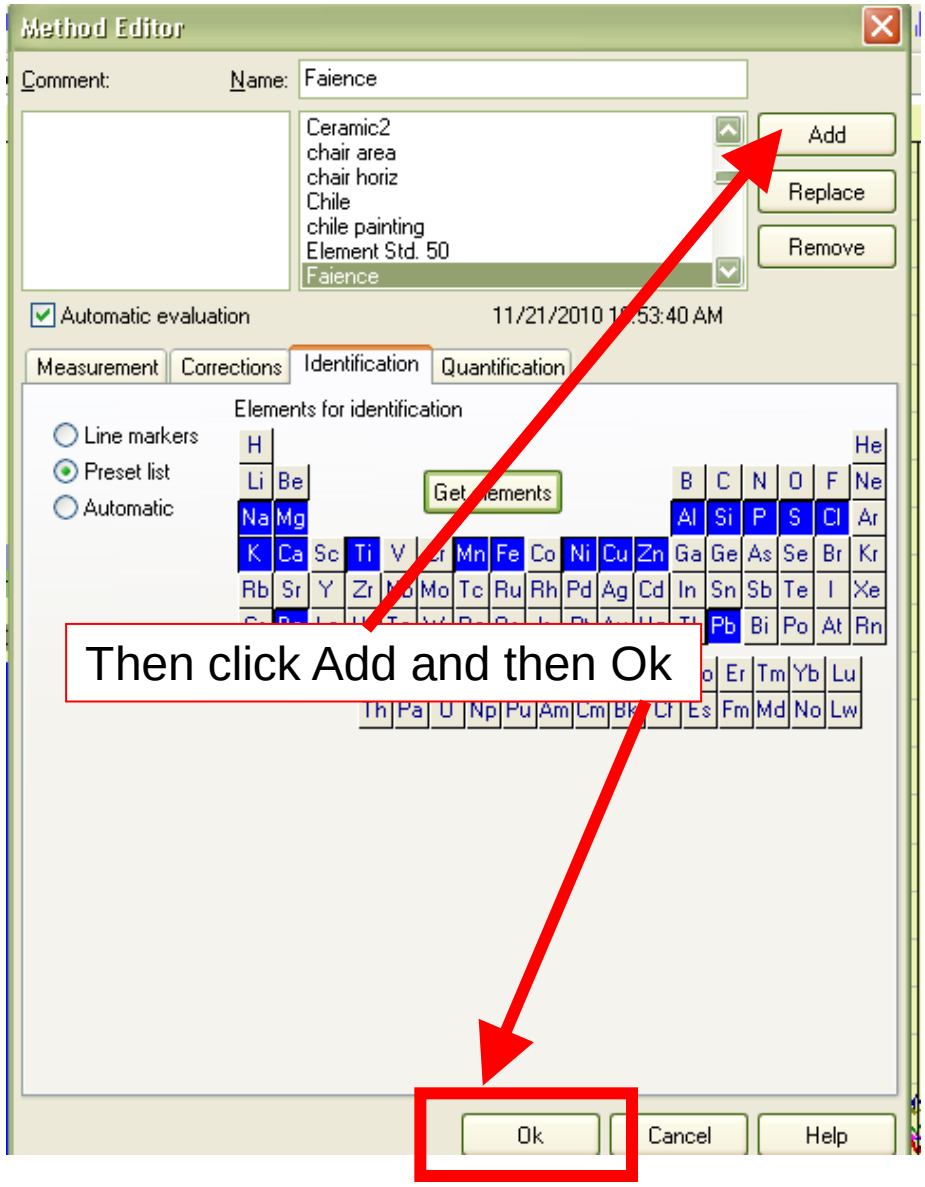


Select “Preset list” and then click on “Get elements” to get the elements you identified in your spectrum to make sure all of your elements highlighted on this table are analyzed every time you use this method.

Then do the following



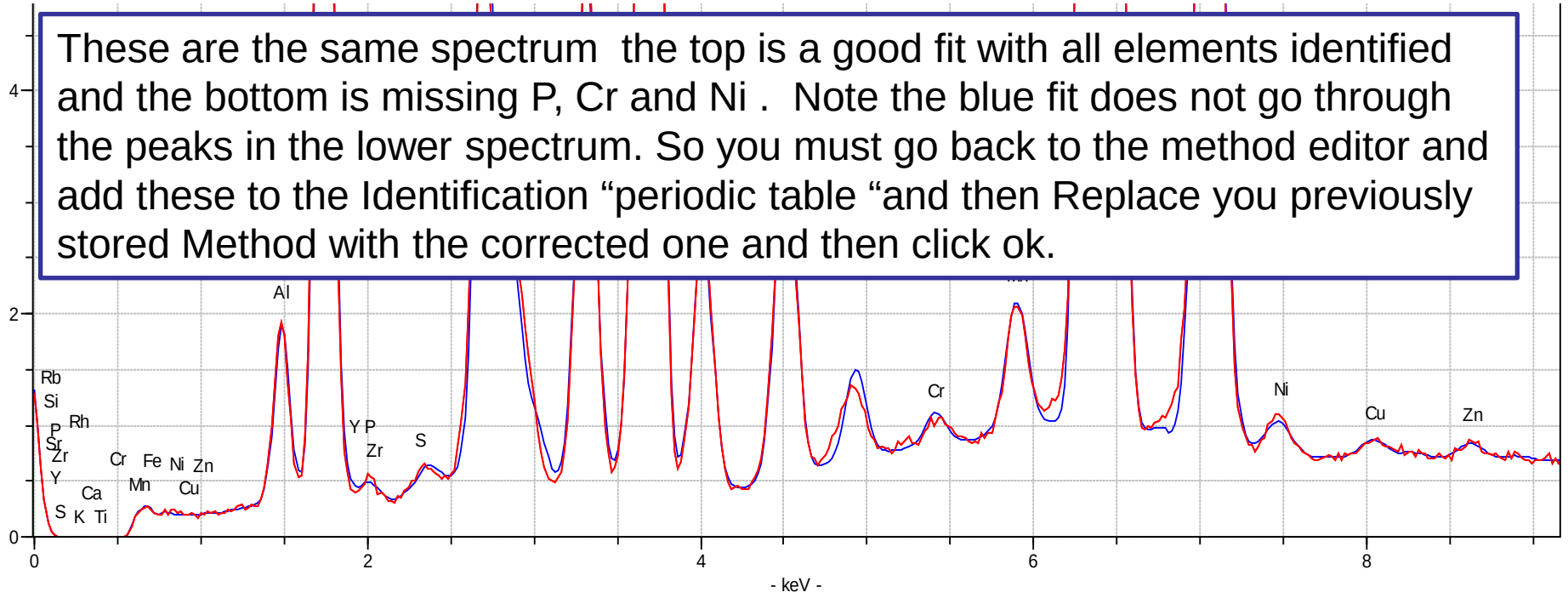
d,

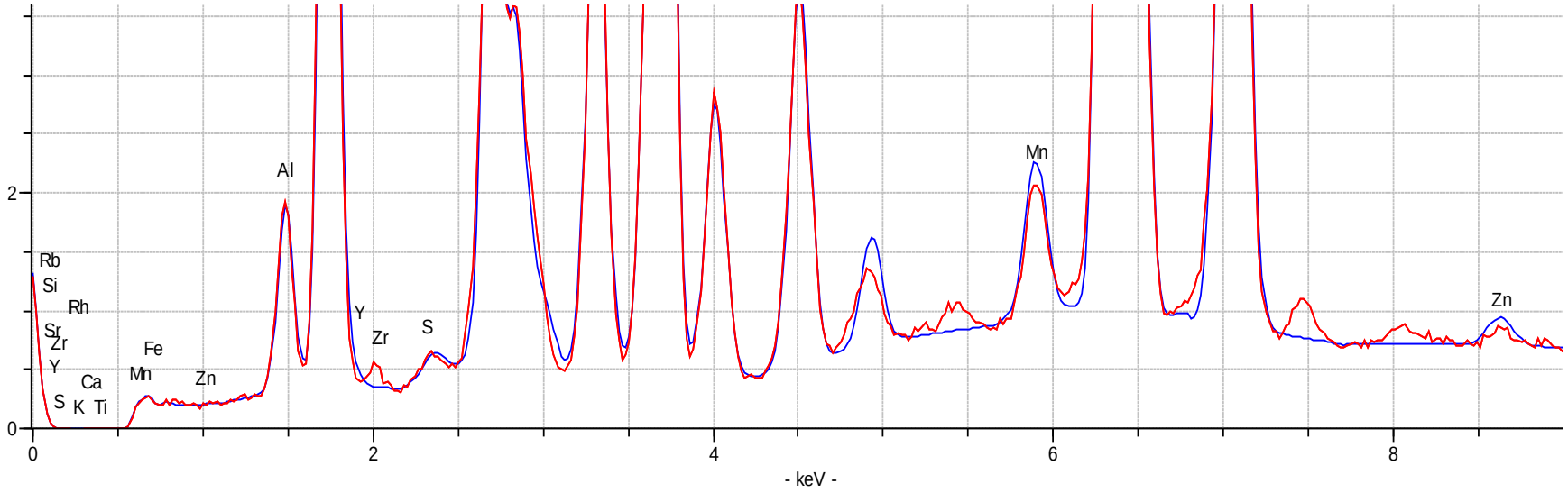


Using Artax for qualitative analysis

1. Create txt files in S1PXRF
2. Open ARTAX and make a new project
3. Choose elements
4. Create Methods file
5. Check the method!
6. Deconvolution of spectrum
   - Export results

These are the same spectrum the top is a good fit with all elements identified and the bottom is missing P, Cr and Ni . Note the blue fit does not go through the peaks in the lower spectrum. So you must go back to the method editor and add these to the Identification “periodic table “and then Replace you previously stored Method with the corrected one and then click ok.





Using Artax for qualitative analysis

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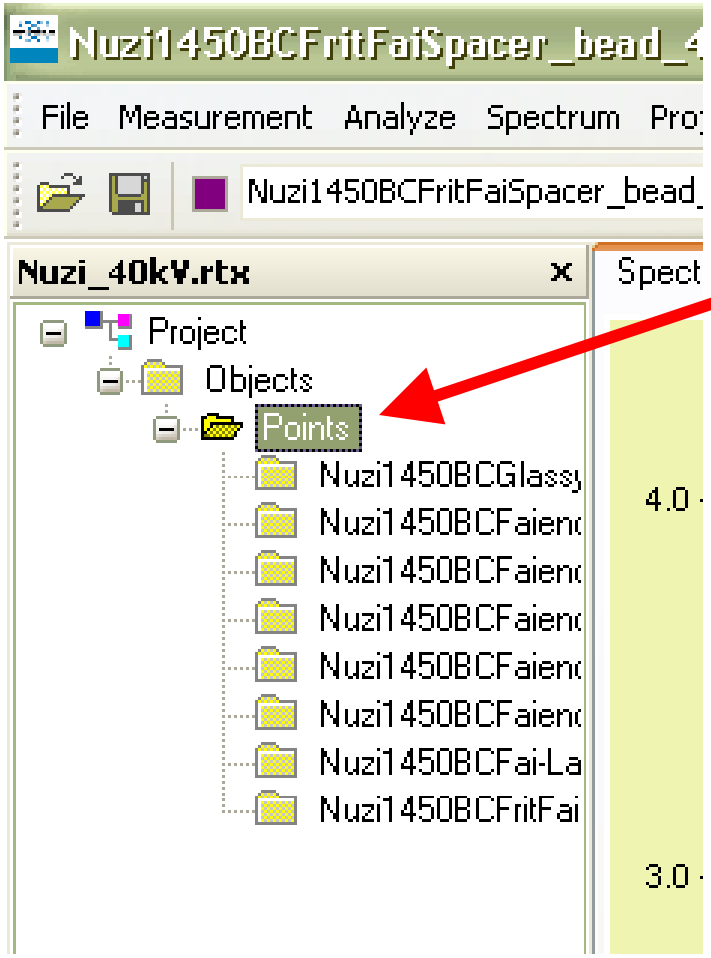
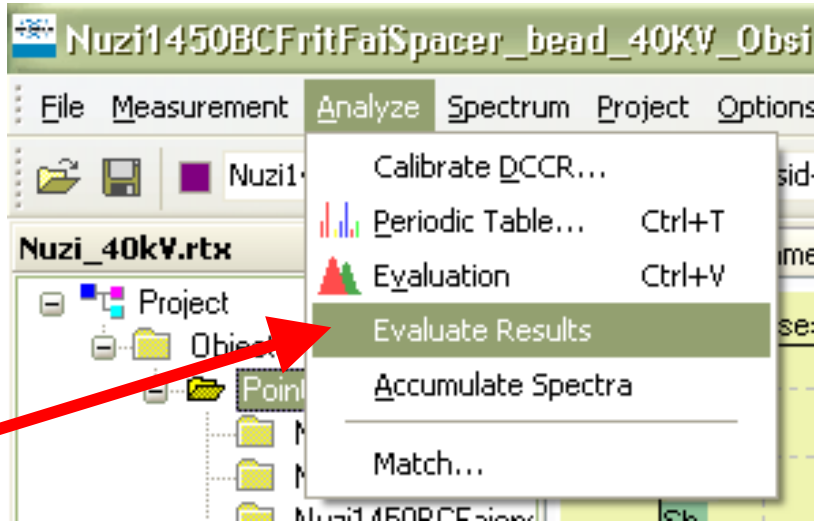
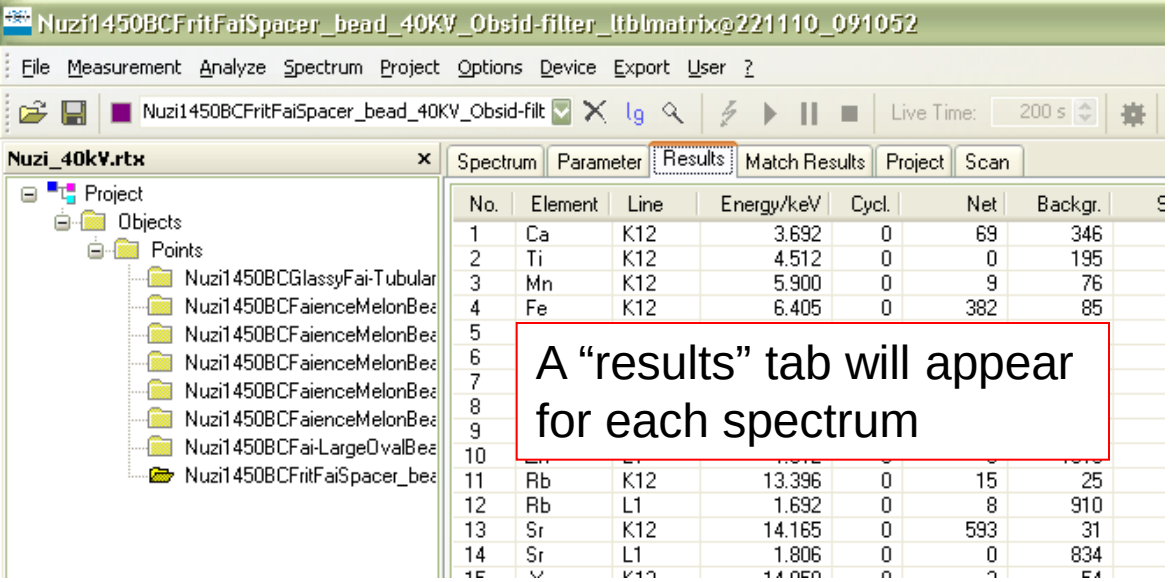


Make sure that the Points folder is highlighted

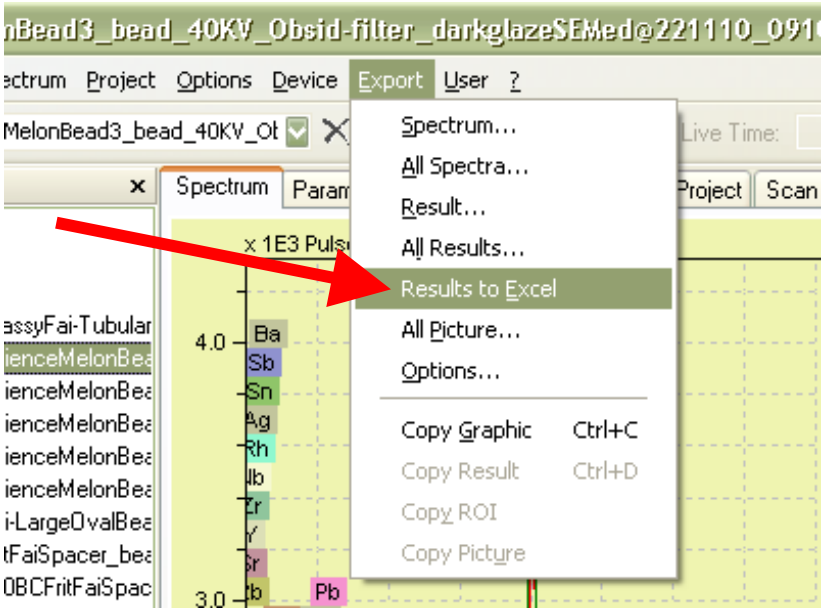


Then select Analyze and Evaluate Results



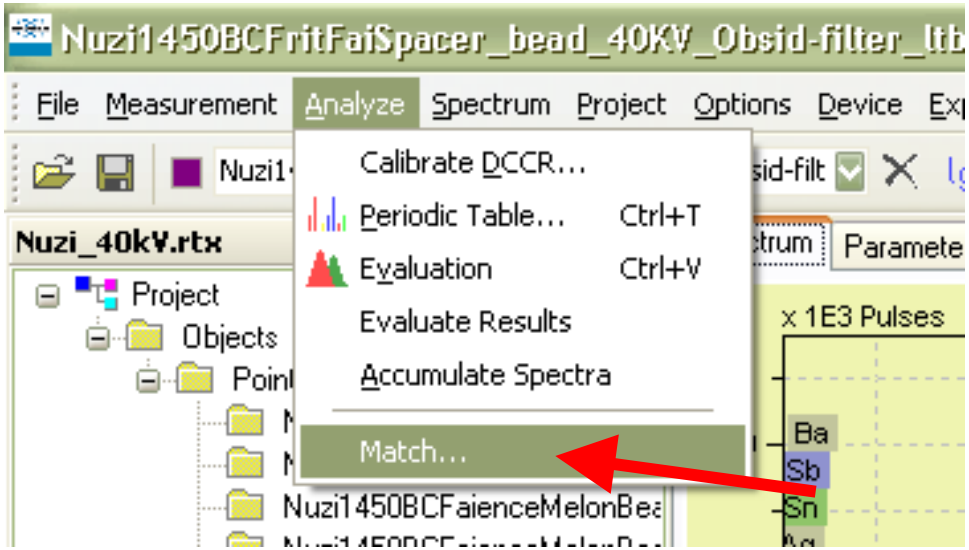
Export the results to excel. This will create a file (you select the name) with one worksheet labeled “Points.” All of your data are listed in this this worksheet. If this worksheet is blank, check the following:

1. All spectra are in the Points node (with capitol “P”)
2. You highlighted the Points folder before Analyzing data
3. There is a results file present for each spectrum



Using Artax for qualitative analysis

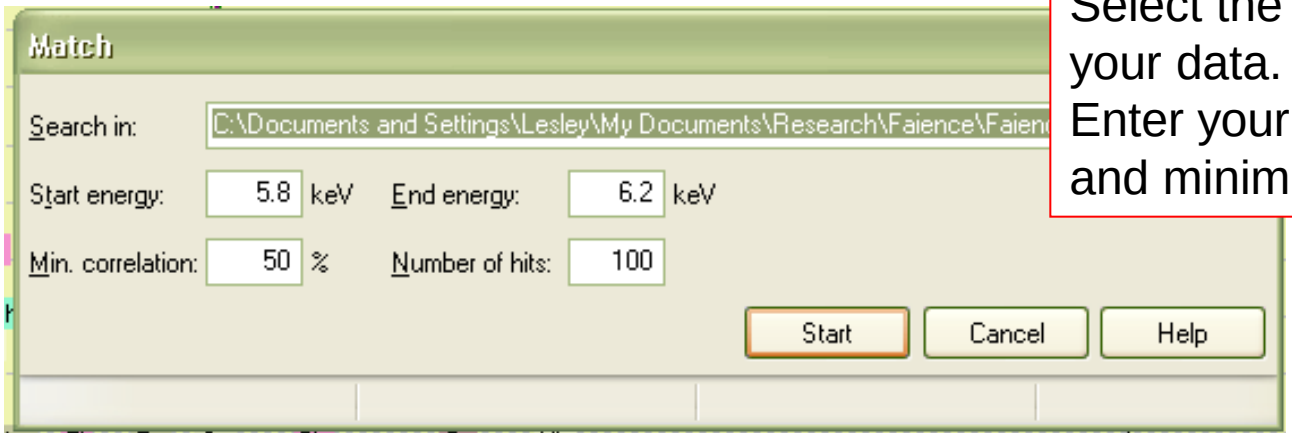
1. Create txt files in S1PXRF
2. Open ARTAX and make a new project
3. Choose elements
4. Create Methods file
5. Deconvolution of spectrum
   - Export results
6. Match peaks



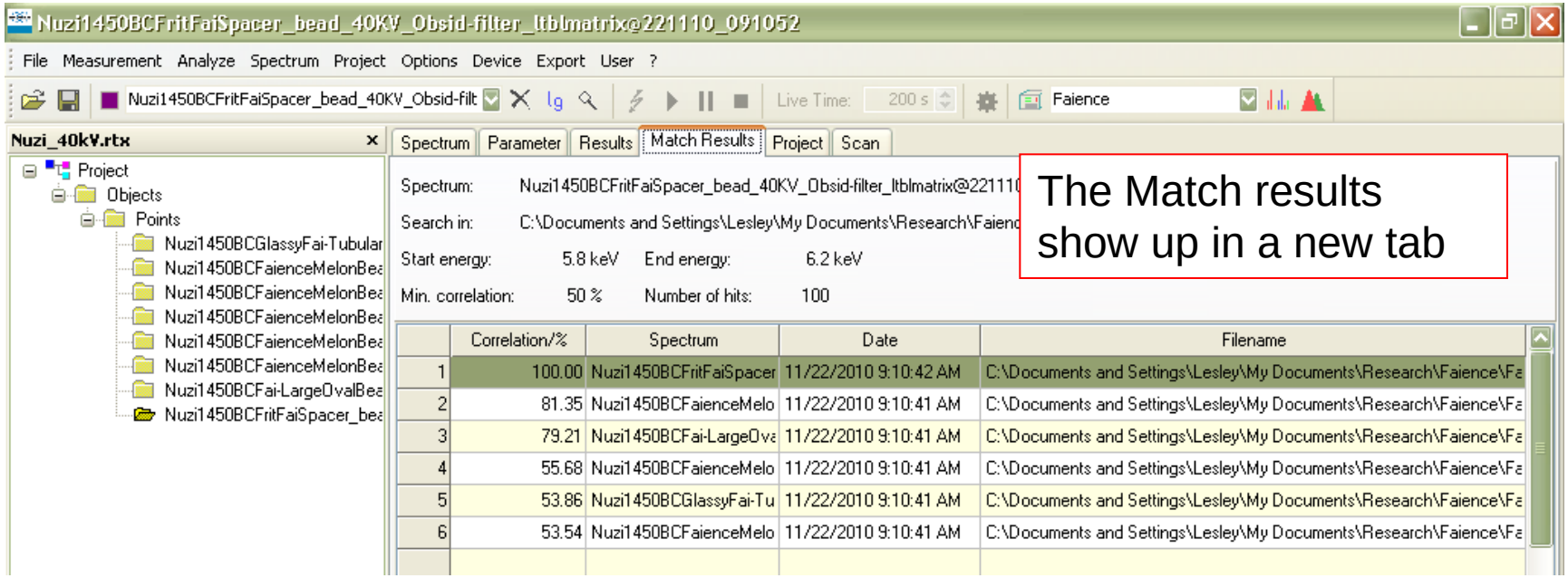
You can use the match peaks function in order to compare all of your spectra in a given project to look for a specific element peak. You must do the following before you perform the Match peak function:

1. All spectra for comparison must be in the same folder.
2. All spectra for comparison must be in a saved project file and the project must be in the same folder as the raw spectra data (txt files).
3. You must know your energy range of interest for which ever element you want to compare.

A new window will open



Select the folder will all of your data.
Enter your energy range and minimum correlation



The Match results show up in a new tab

Be careful

- Use similar size samples (infinitely thick, or normalize to background before doing other comparisons)
- Make sure your deconvolution matches your actual spectrum (don’t ignore any of the real peaks!)
- Don’t ignore half of your energy lines (i.e., both Kα and Kβ are important!)