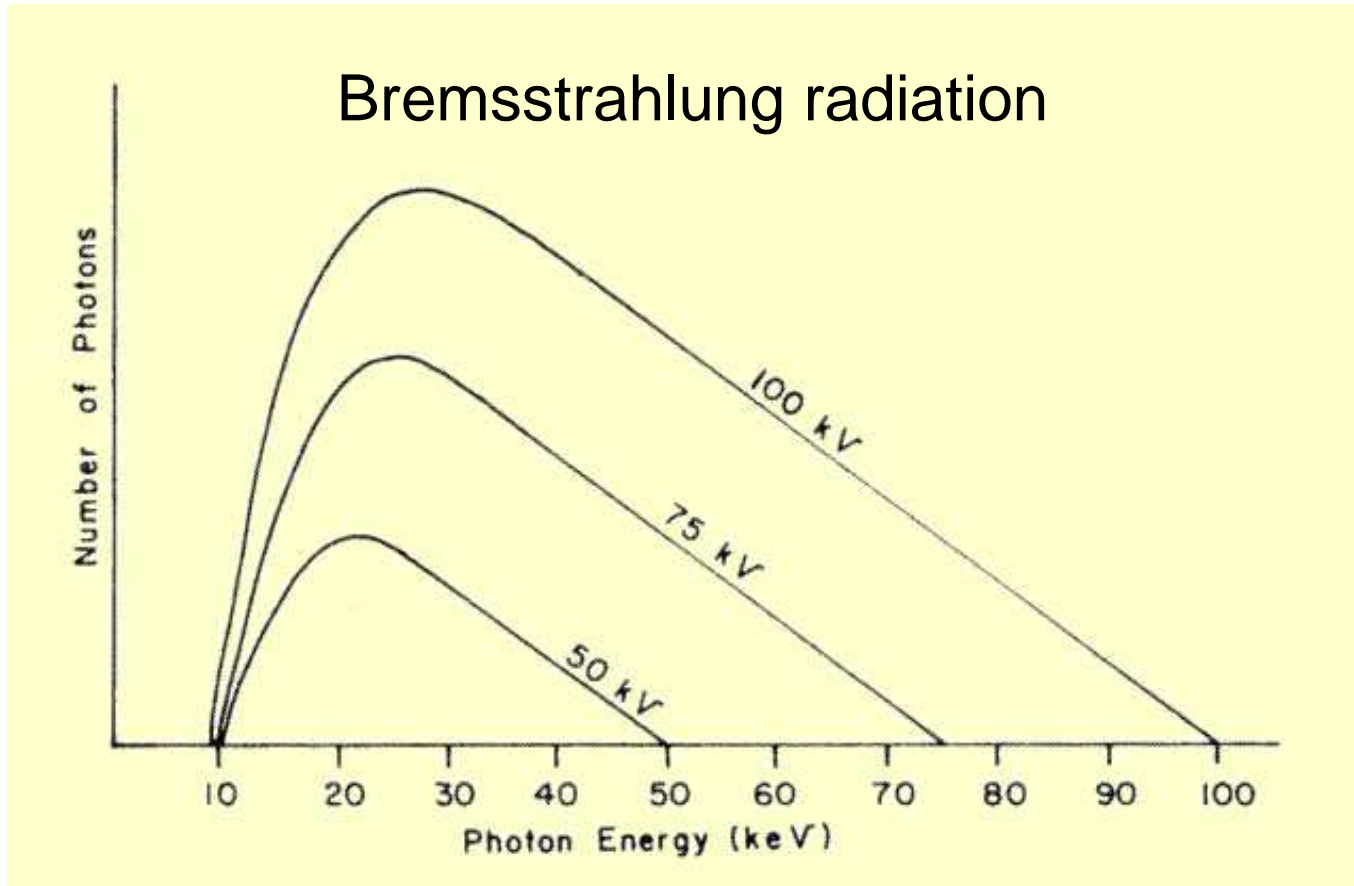


Qualitative analysis tutorial for Tracer III SD and V+ data

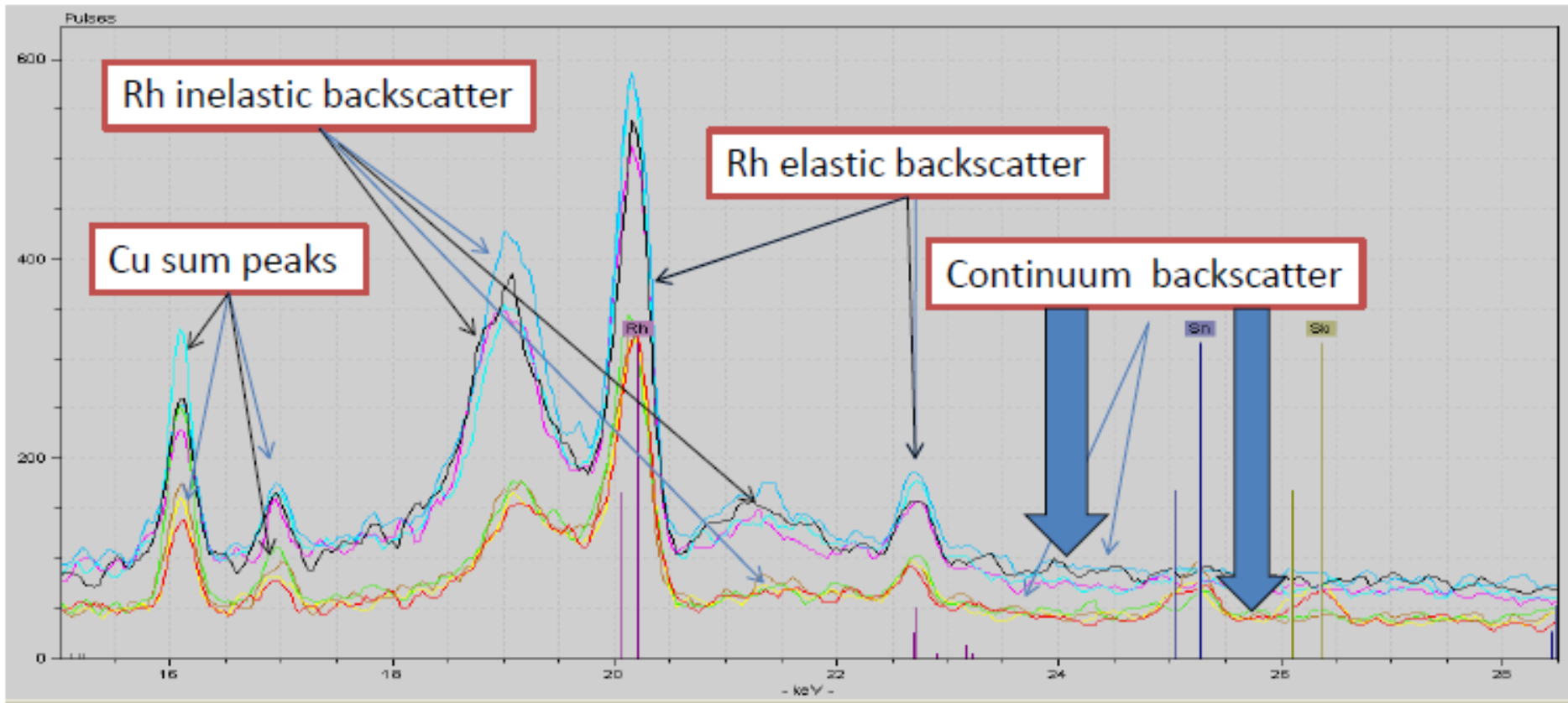
Outline

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

What does the spectrum mean?



What does the spectrum mean?

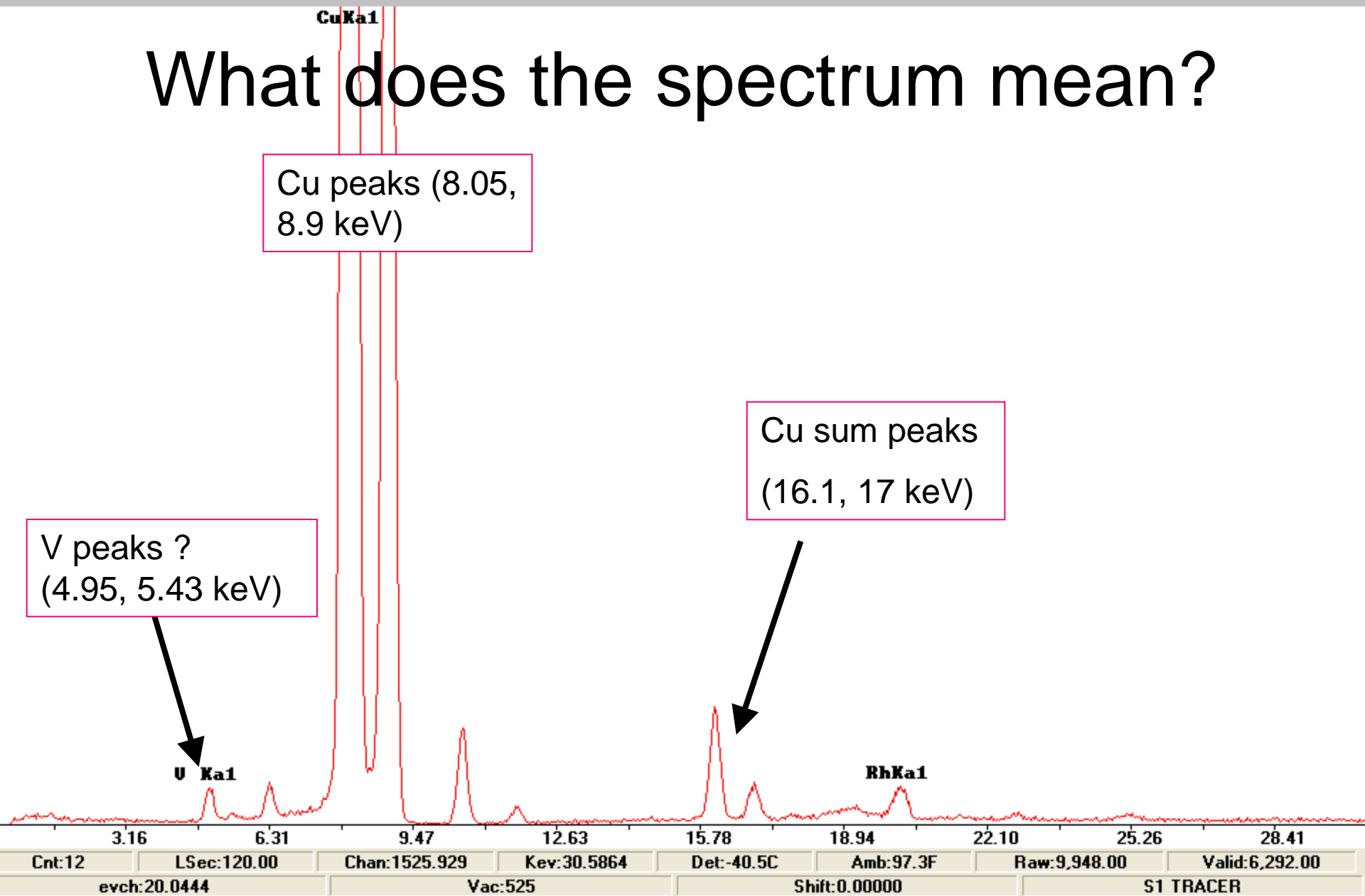


What does the spectrum mean?

Cu peaks (8.05, 8.9 keV)

Cu sum peaks (16.1, 17 keV)

V peaks ? (4.95, 5.43 keV)



V Ka1

RhKa1

Cnt:12 LSec:120.00 Chan:1525.929 Kev:30.5864 Det:-40.5C Amb:97.3F Raw:9,948.00 Valid:6,292.00
evch:20.0444 Vac:525 Shift:0.00000 S1 TRACER

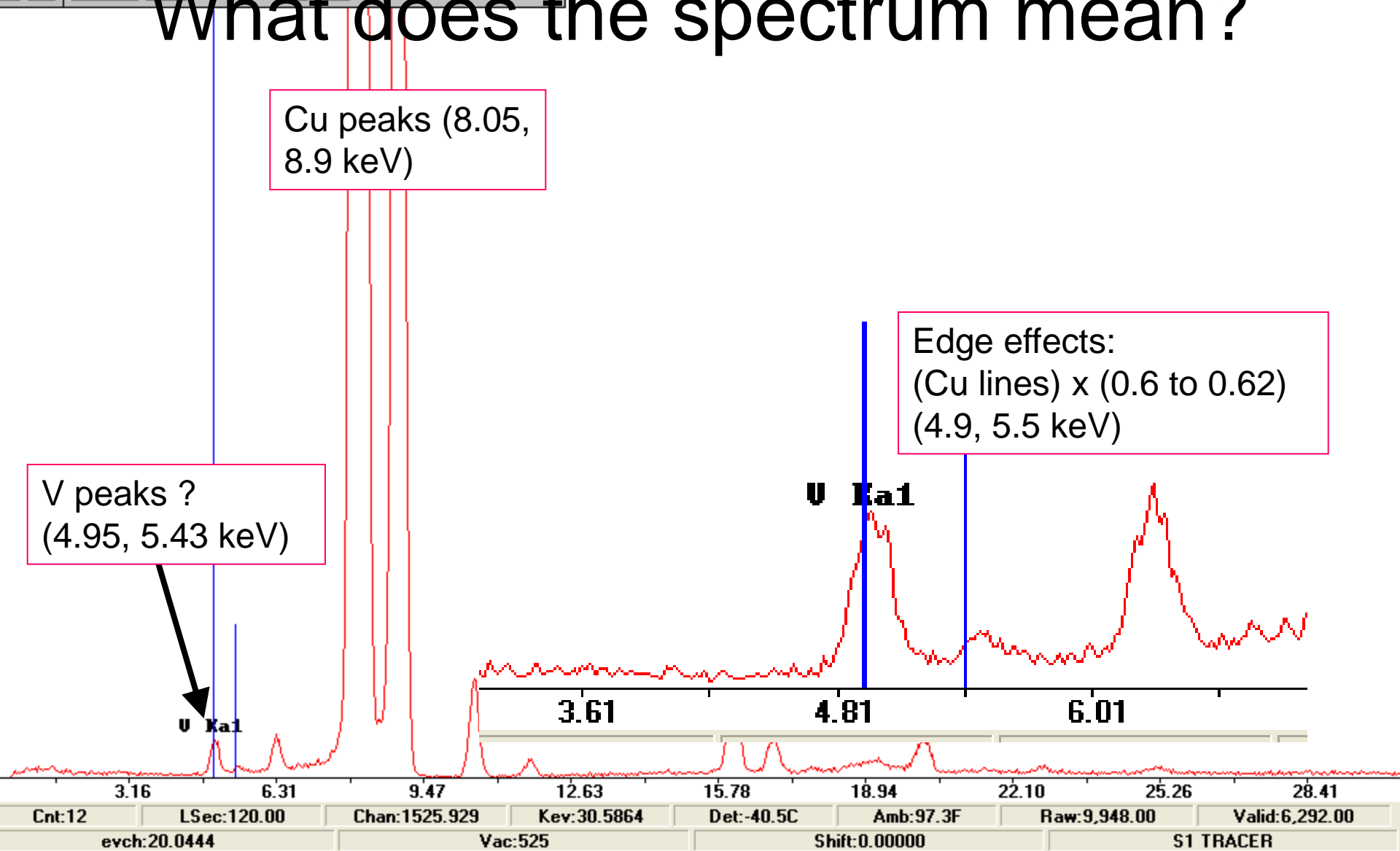
Copper alloy

What does the spectrum mean?

Cu peaks (8.05, 8.9 keV)

Edge effects:
(Cu lines) x (0.6 to 0.62)
(4.9, 5.5 keV)

V peaks ?
(4.95, 5.43 keV)



Copper alloy

What does the spectrum mean?

Cu peaks (8.05, 8.9 keV)

Edge effects:
(Cu lines) x (0.6 to 0.62)
(4.9, 5.5 keV)

Cu sum peaks
(16.1, 17 keV)

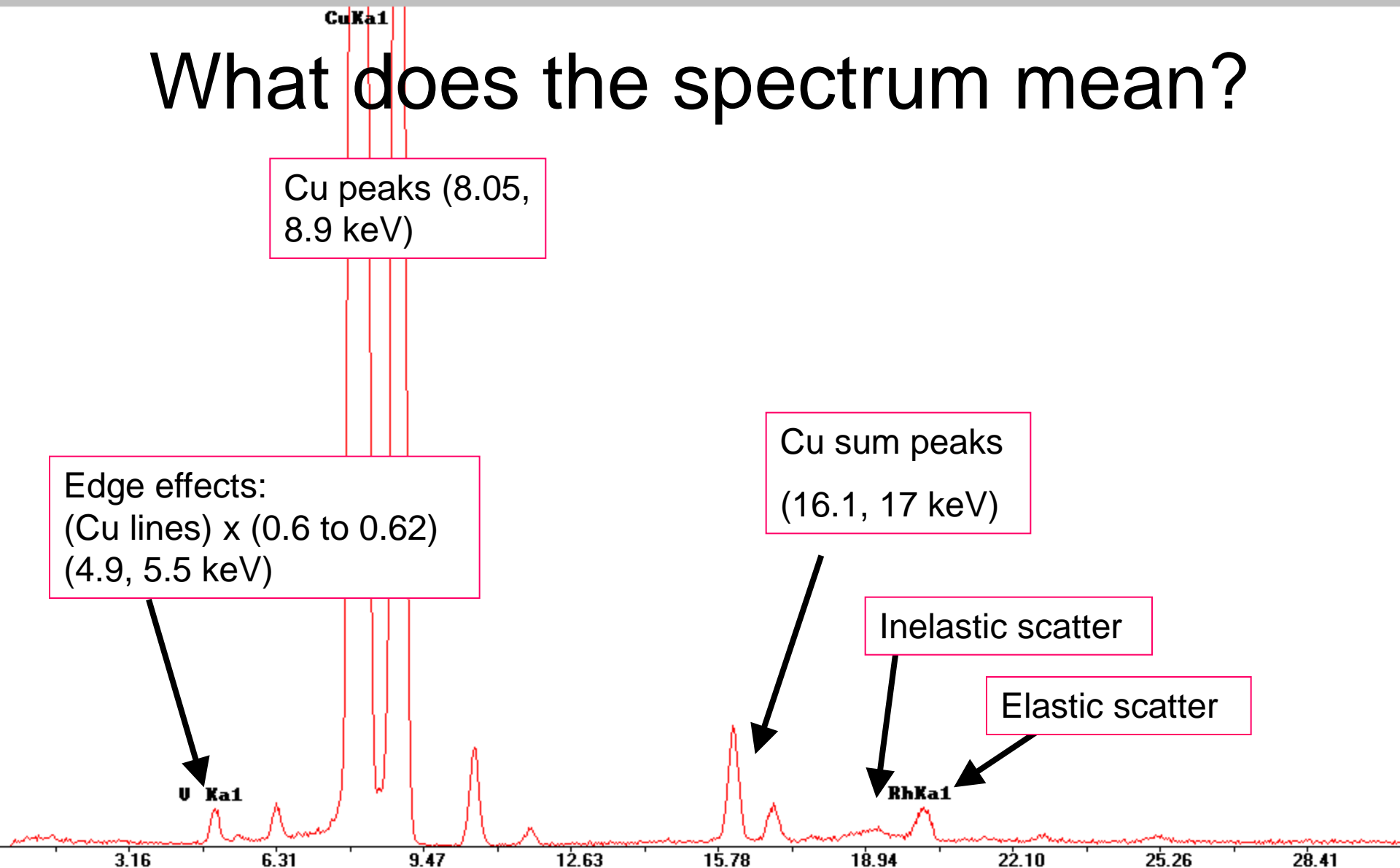
Inelastic scatter

Elastic scatter

U Ka1

RhKa1

CuKa1



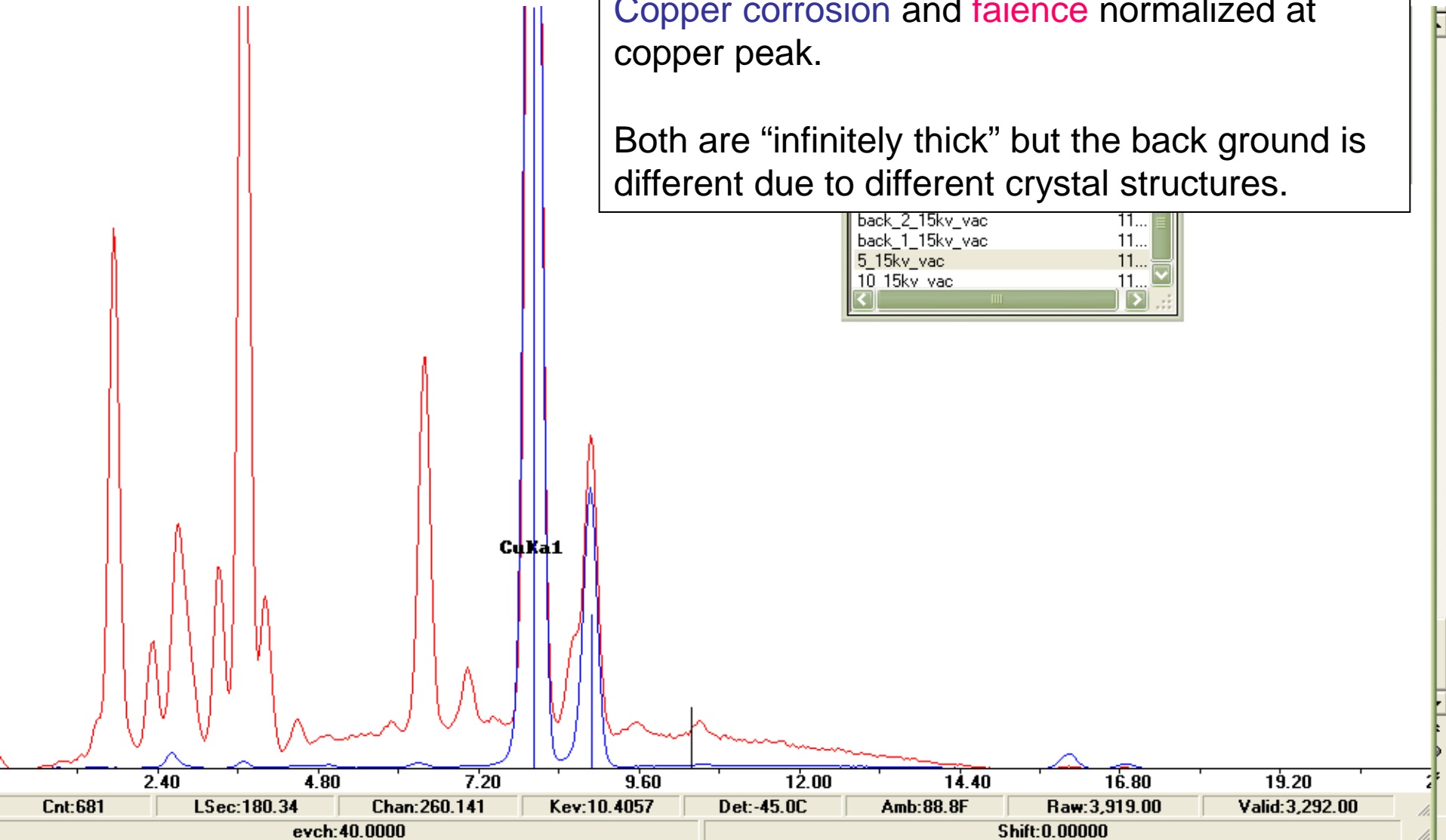
Cnt:12	LSec:120.00	Chan:1525.929	KeV:30.5864	Det:-40.5C	Amb:97.3F	Raw:9,948.00	Valid:6,292.00
evch:20.0444		Vac:525		Shift:0.00000		S1 TRACER	

Copper alloy

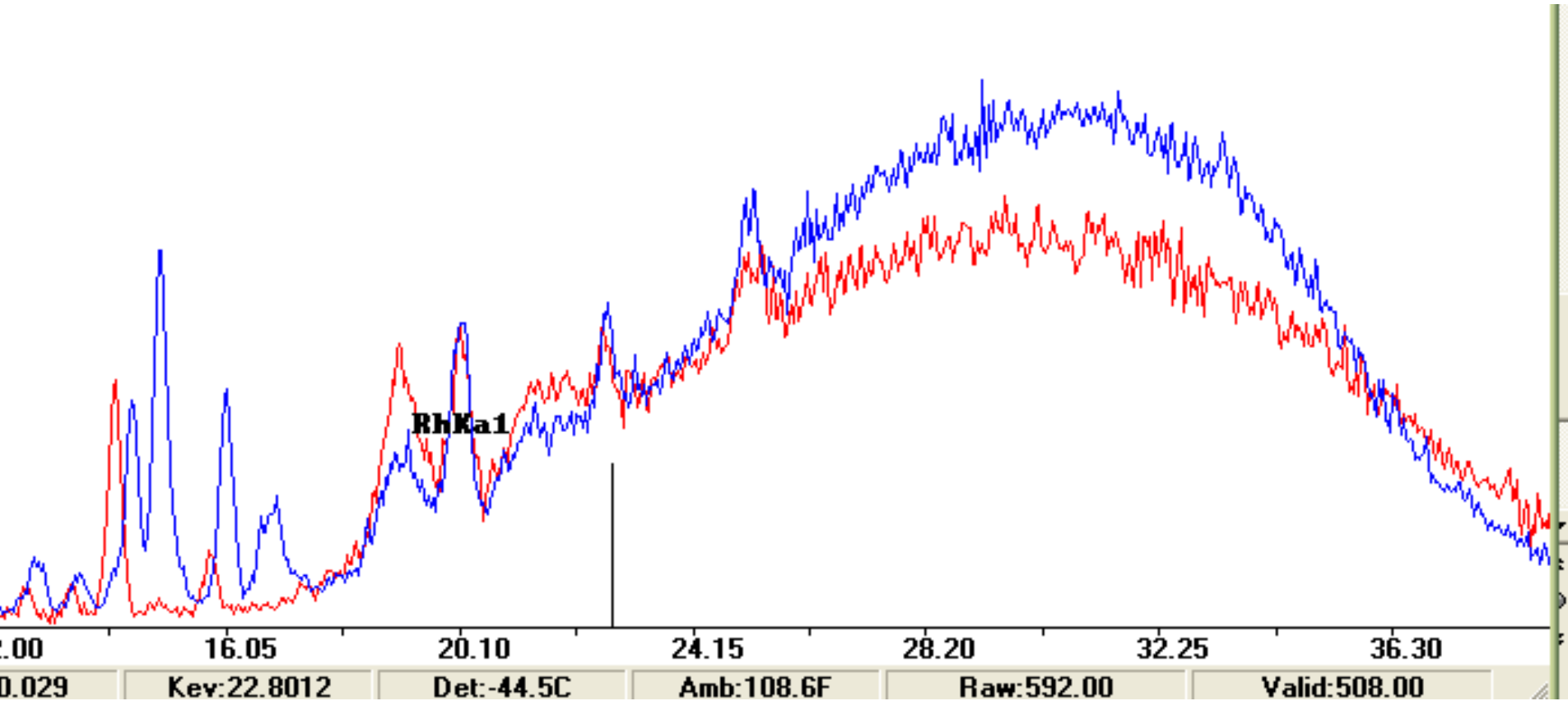
What does the spectrum mean?

Copper corrosion and faience normalized at copper peak.

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



What does the spectrum mean?



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

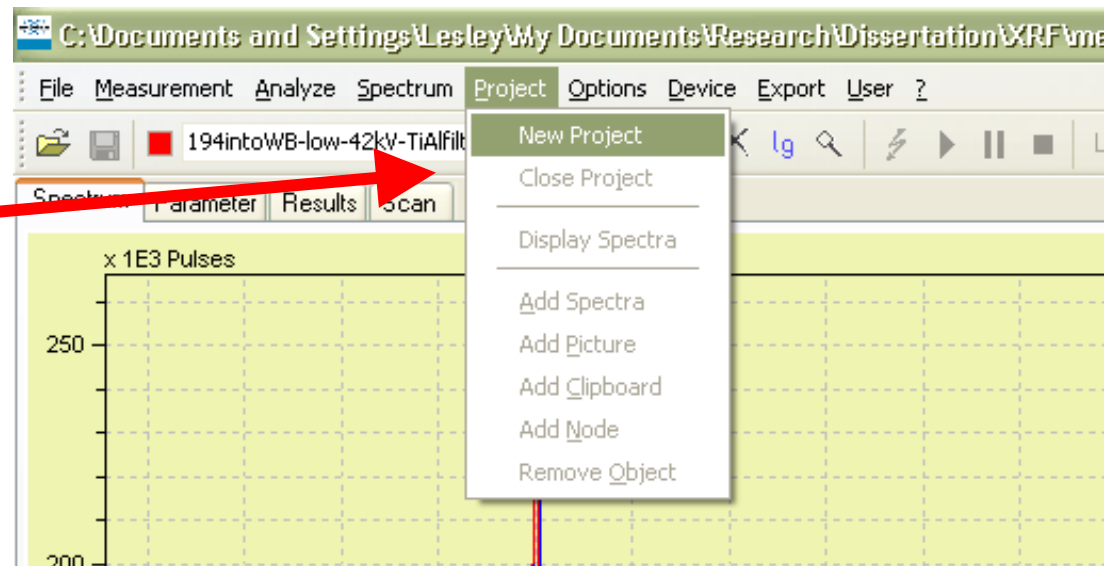
- Click on File and open spectra
- Make sure files of type is on txt
- you can only have 100 spectra on the display at any one time, but you can have up to 4000000 spectra in your Points folder that you do the analysis on.
- So open 100 spectra or less and then add them to the Points folder. Then clear 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.

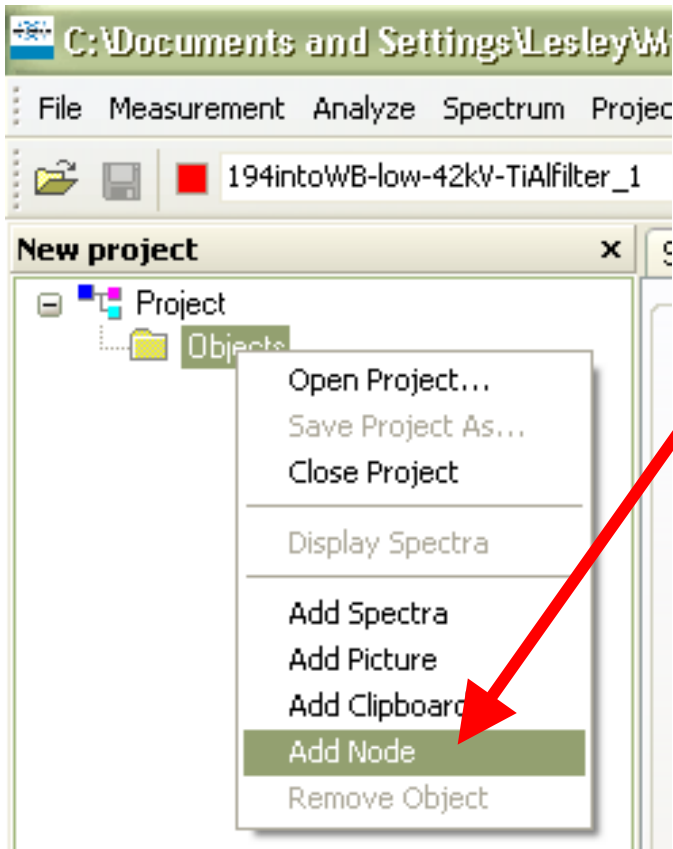
Using Artax for qualitative analysis

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

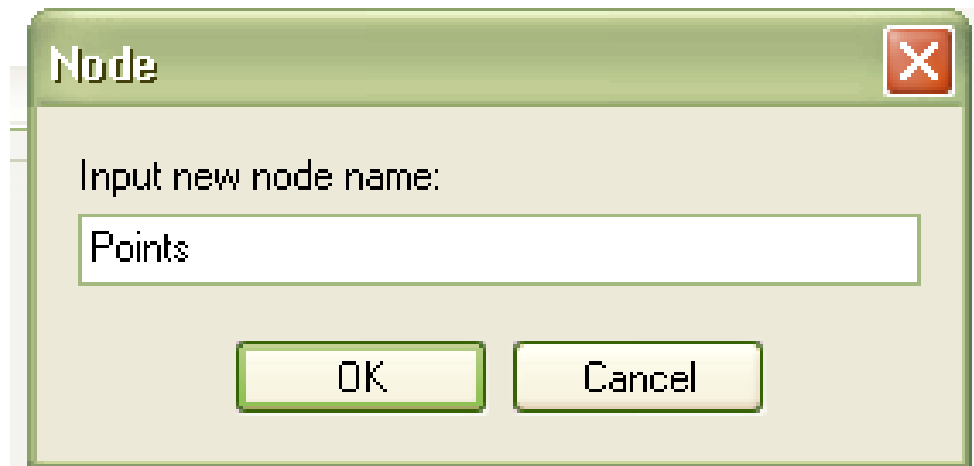


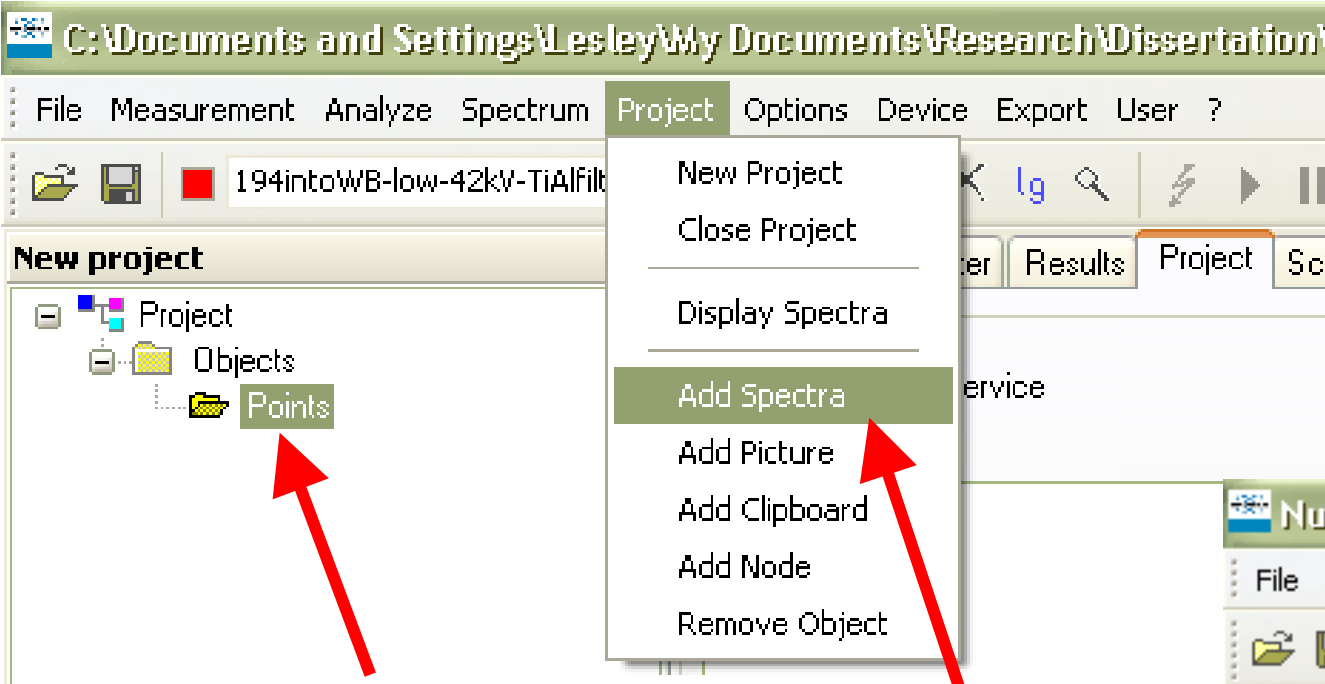


Right click on Objects in the project pane, select Add Node

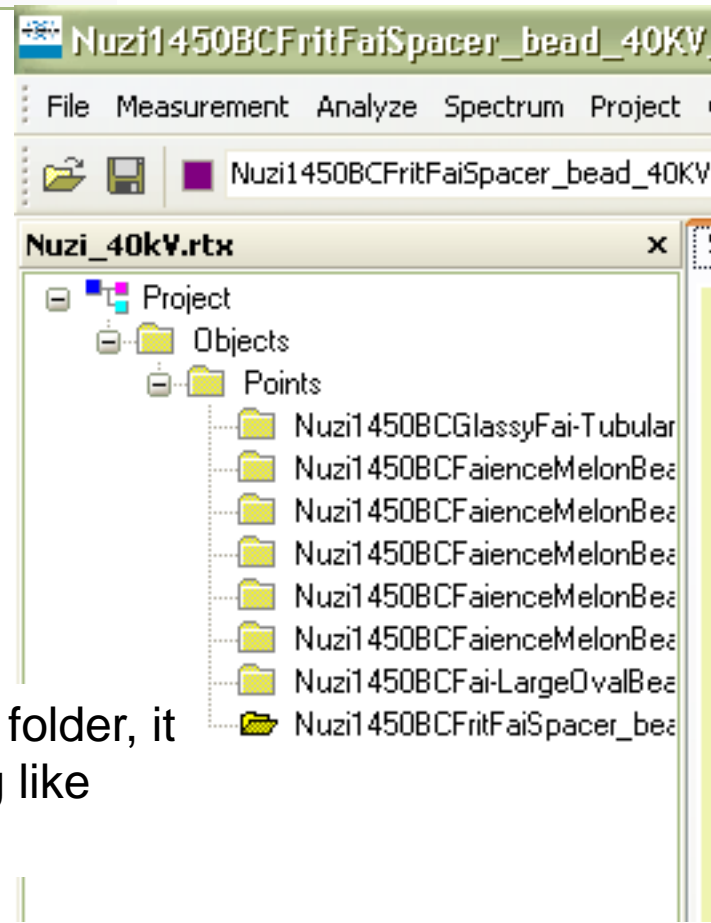
A new window will open

Name the node "Points"
(with capitol P)





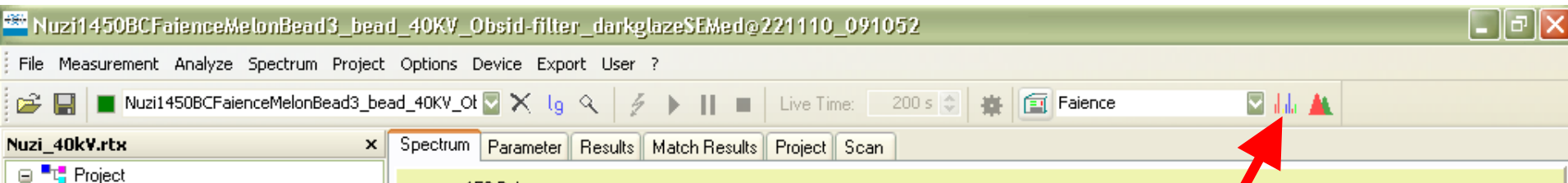
Click on Points folder. Go to Projects and select Add Spectra. All of the opened spectra will be added to this node



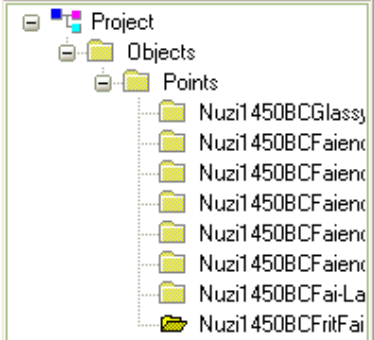
When you expand the folder, it should look something like this.

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



Periodic Table of the Elements

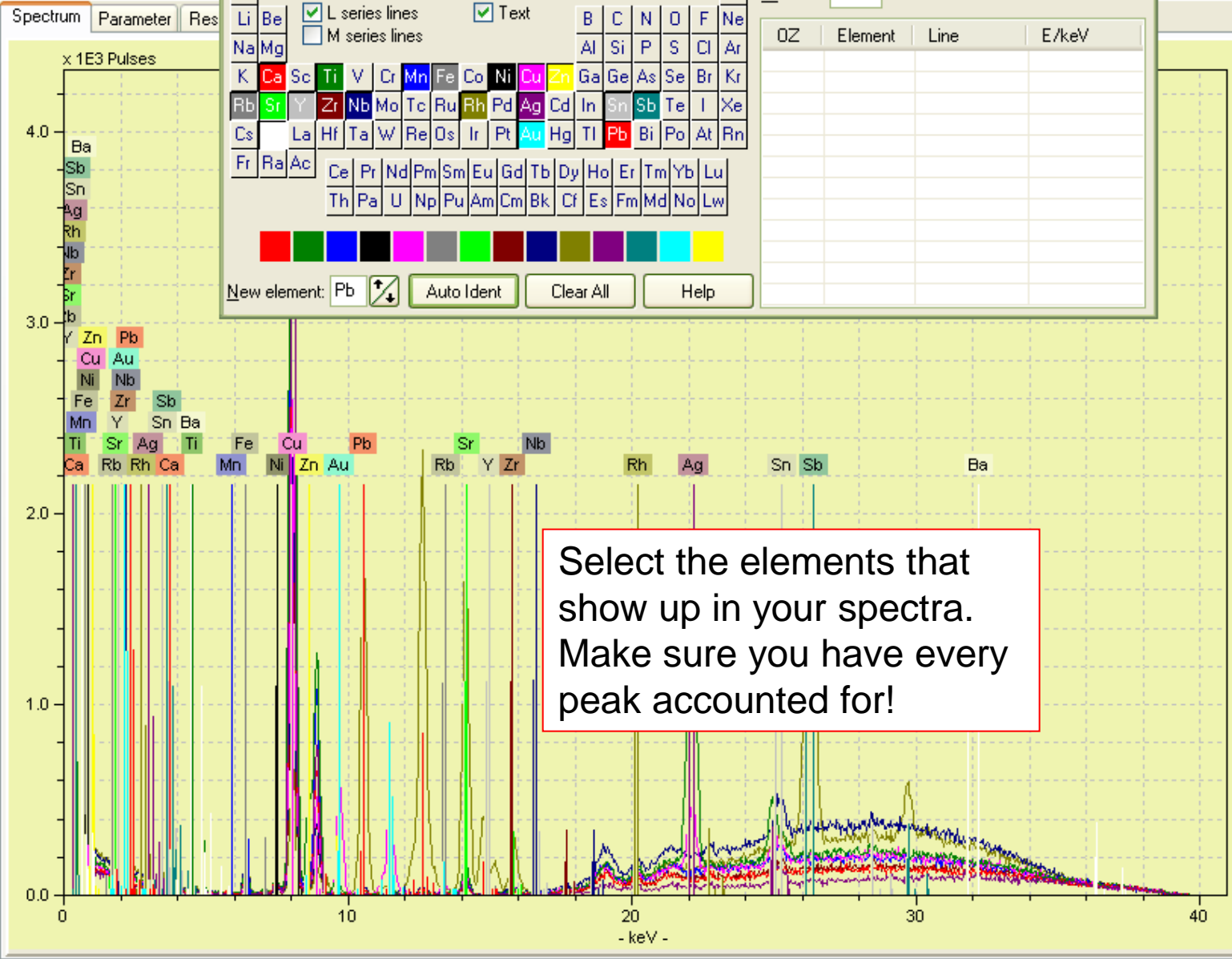
K series lines Lines
 L series lines Text
 M series lines

H	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 La Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn	
Fr Ra Ac	Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
	Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lw

New element: Pb [dropdown] [arrow]
[Auto Ident] [Clear All] [Help]

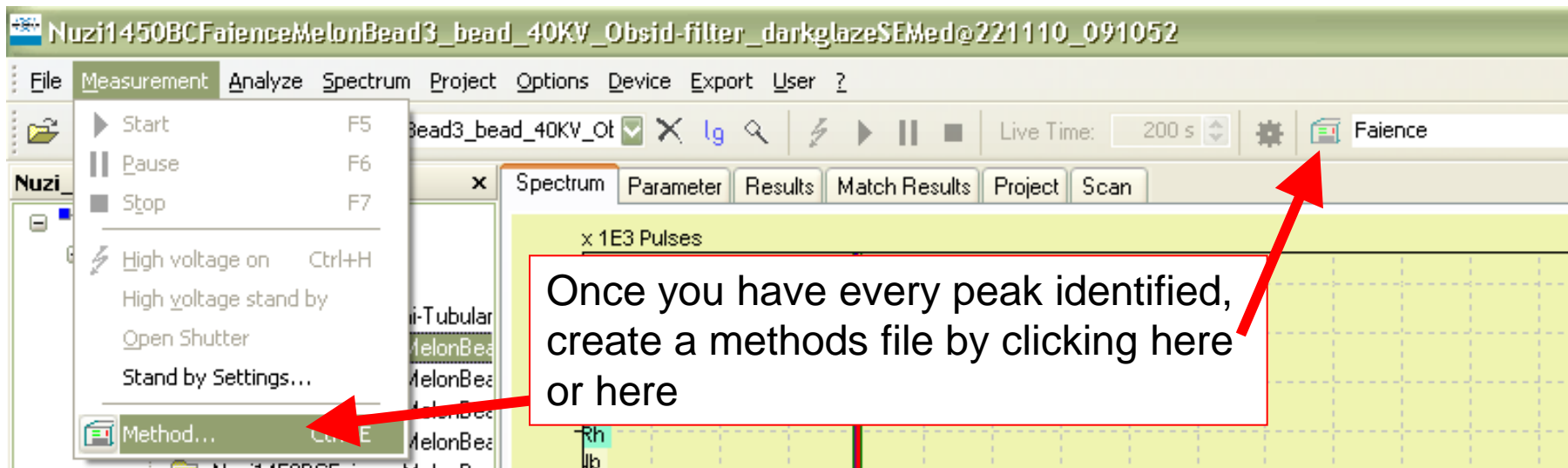
Window: 0.05 keV

OZ	Element	Line	E/keV

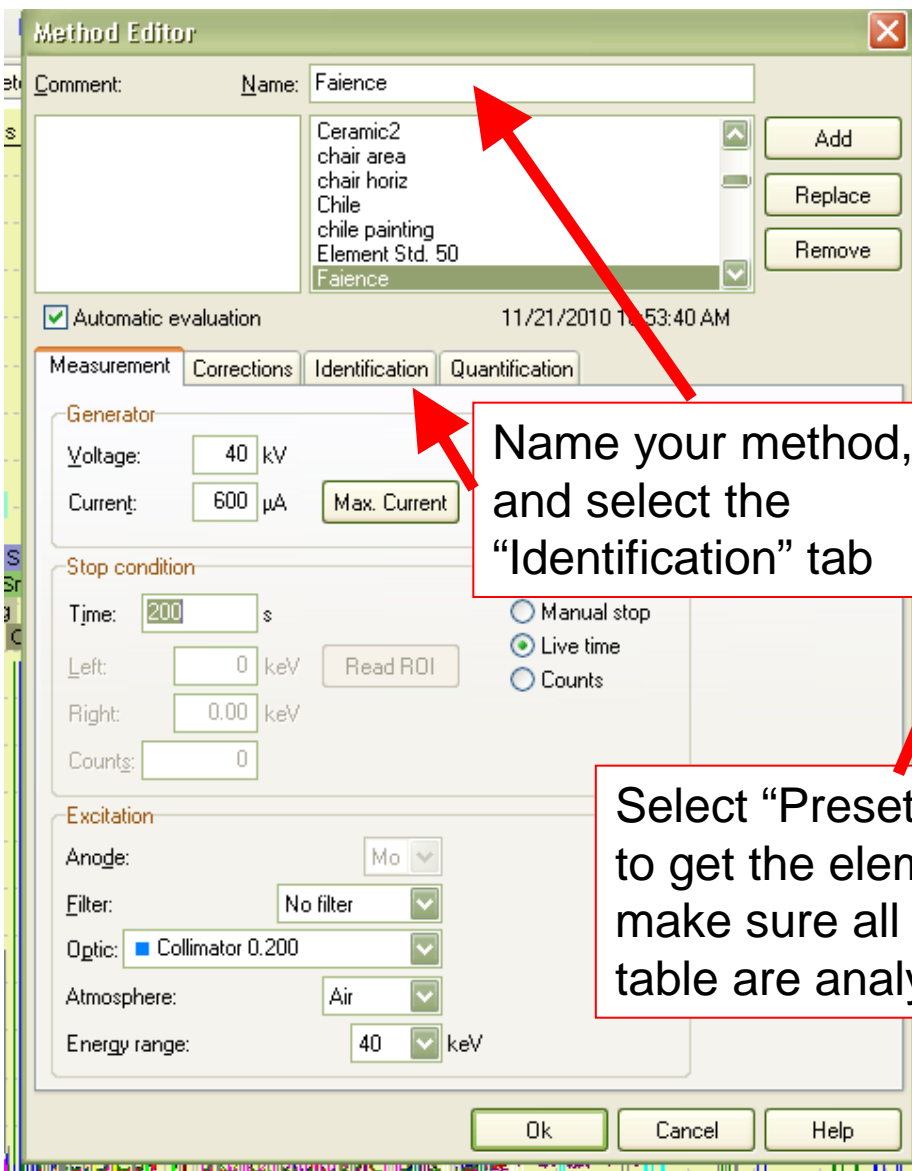


Using Artax for qualitative analysis

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



Method Editor

Comment: Name:

Ceramic2
chair area
chair horiz
Chile
chile painting
Element Std. 50
Faience

Automatic evaluation 11/21/2010 10:53:40 AM

Measurement Corrections **Identification** Quantification

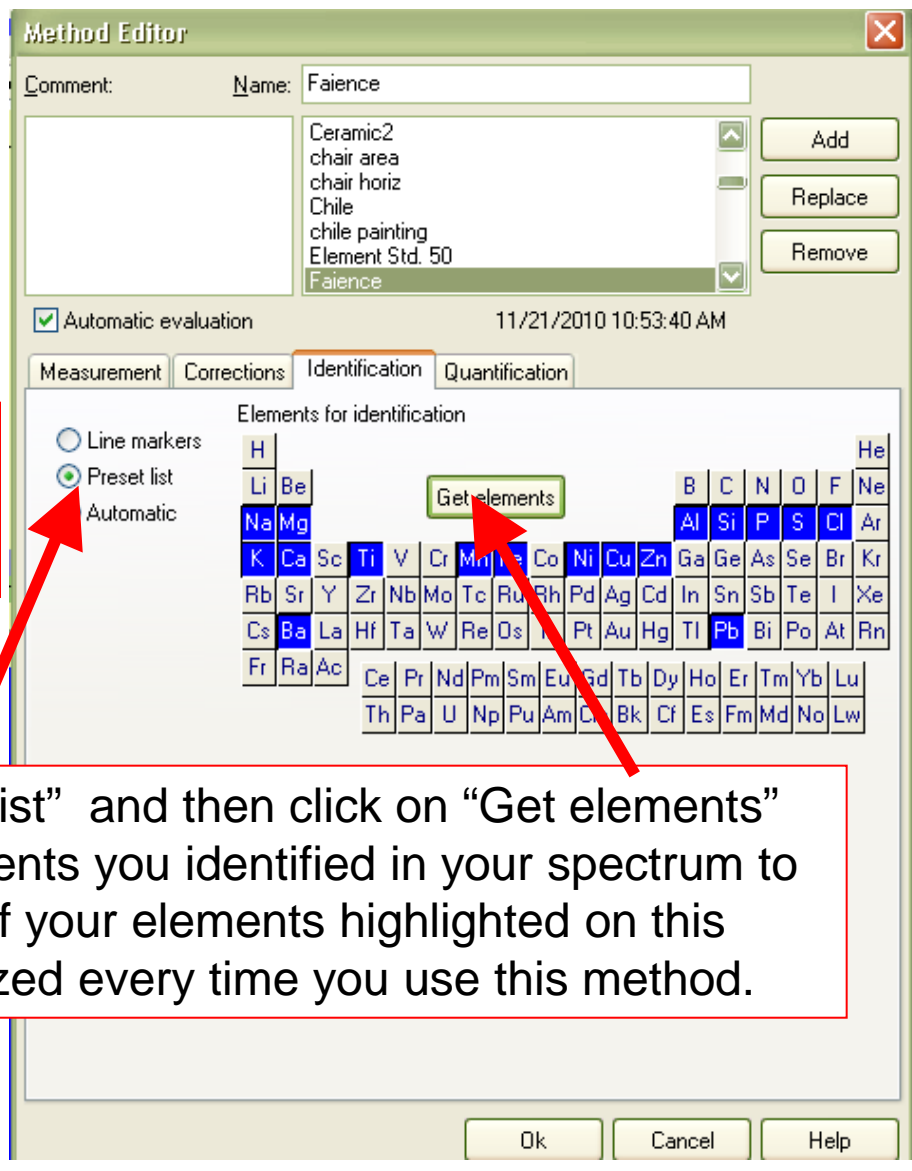
Generator
Voltage: kV
Current: μ A

Stop condition
Time: s
Left: keV
Right: keV
Counts:

Manual stop
 Live time
 Counts

Excitation
Anode:
Filter:
Optic:
Atmosphere:
Energy range: keV

Name your method,
and select the
“Identification” tab



Method Editor

Comment: Name:

Ceramic2
chair area
chair horiz
Chile
chile painting
Element Std. 50
Faience

Automatic evaluation 11/21/2010 10:53:40 AM

Measurement Corrections **Identification** Quantification

Line markers
 Preset list
 Automatic

Elements for identification

H																			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		Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra	Ac																	
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw			

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

Method Editor

Comment: Name:

left pilgrim behind eye
lo e U Wis
Low Bryant
manuell
melbourne
meteorites stone
metSU 0093.yf

Automatic evaluation 03/01/2011 3:45:45 AM

Measurement Corrections Identification Quantification

Escape

 Background Cycles: Start: keV End: keV

Select "Corrections" and check the Escape and Background box and choose 5 to 10 cycles and then the energy range in your spectrum you wish to fit

d,

Method Editor

Comment: Name:

Ceramic2
chair area
chair horiz
Chile
chile painting
Element Std. 50
Faience

Automatic evaluation 11/21/2010 11:53:40 AM

Measurement Corrections Identification Quantification

Elements for identification

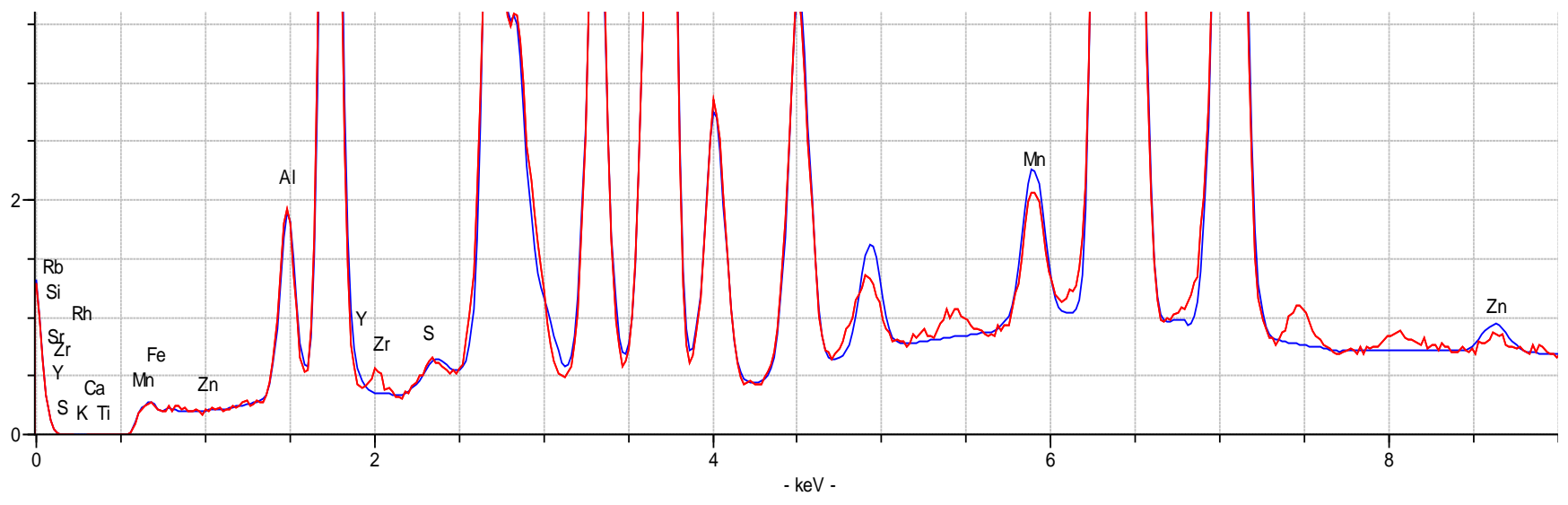
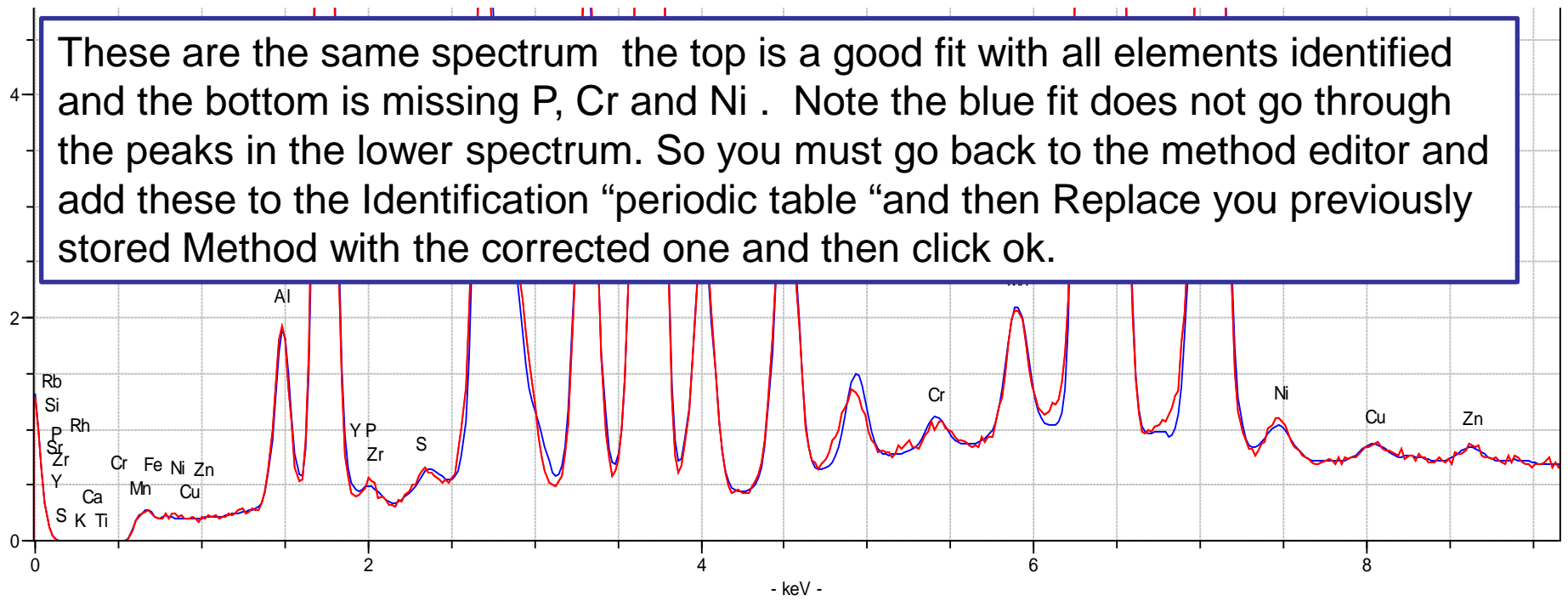
Line markers
 Preset list
 Automatic

H																			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	

Using Artax for qualitative analysis

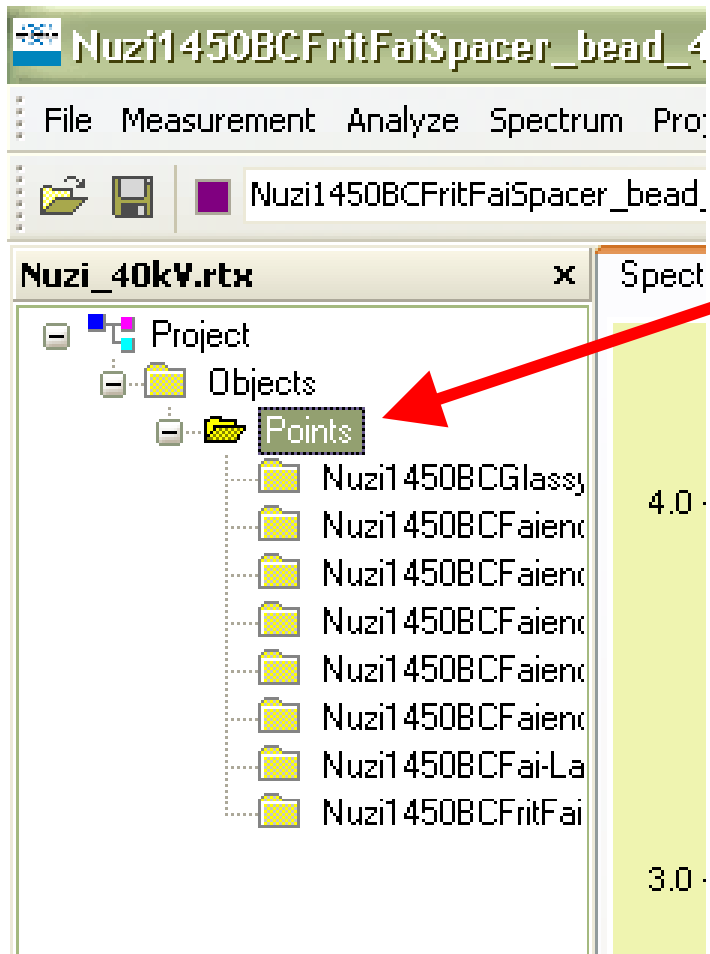
1. Create txt files in S1PXRF
2. Open ARTAX and make a new project
3. Choose elements
4. Create Methods file
5. Check the method!
6. Deconvolution of spectrum
 - Export results

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.



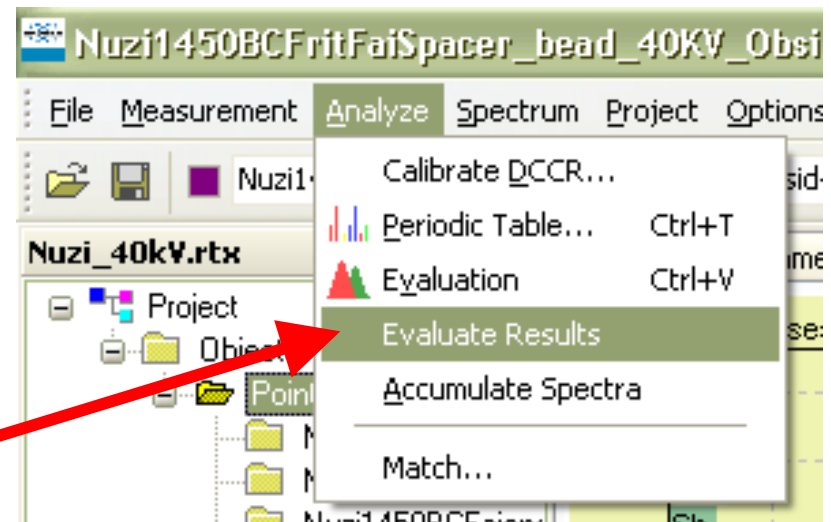
Using Artax for qualitative analysis

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



Make sure that the Points folder is highlighted

Then select Analyze and Evaluate Results



Nuzi1450BCFritFaiSpacer_bead_40KV_Obsid-filter_tlbmatrix@221110_091052

File Measurement Analyze Spectrum Project Options Device Export User ?

Nuzi1450BCFritFaiSpacer_bead_40KV_Obsid-filt lg Live Time: 200 s

Nuzi_40kV.rtx

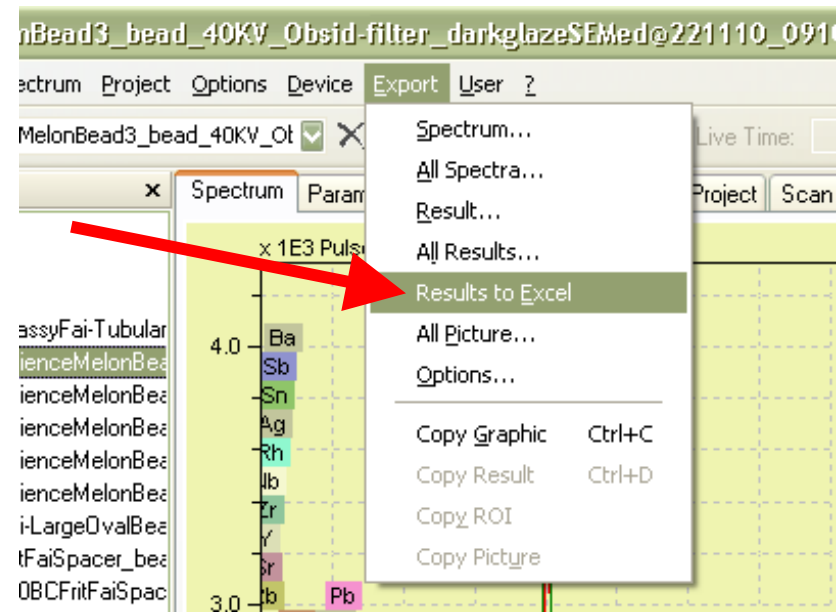
Spectrum Parameter Results Match Results Project Scan

No.	Element	Line	Energy/keV	Cycl.	Net	Backgr.
1	Ca	K12	3.692	0	69	346
2	Ti	K12	4.512	0	0	195
3	Mn	K12	5.900	0	9	76
4	Fe	K12	6.405	0	382	85
5						
6						
7						
8						
9						
10						
11	Rb	K12	13.396	0	15	25
12	Rb	L1	1.692	0	8	910
13	Sr	K12	14.165	0	593	31
14	Sr	L1	1.806	0	0	834
15						

A "results" tab will appear for each spectrum

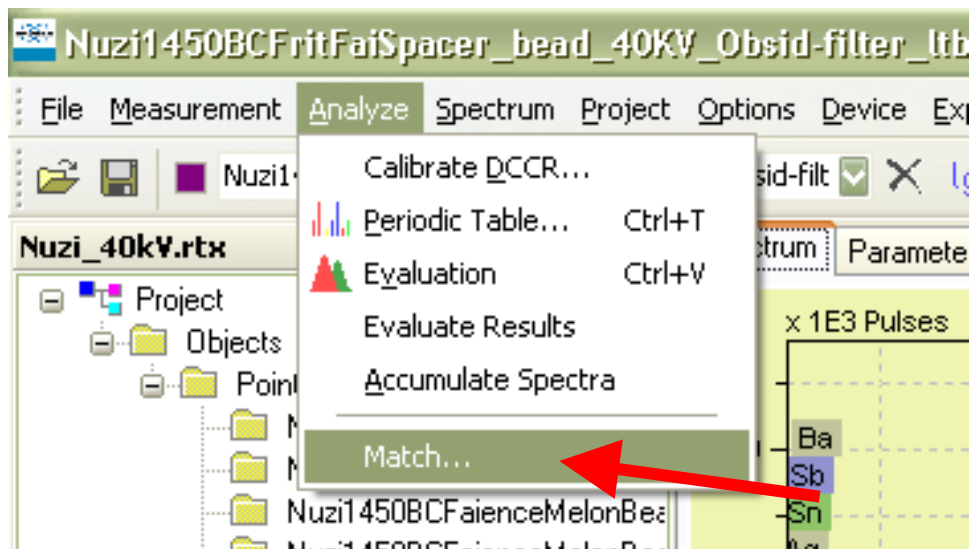
Export the results to excel. This will create a file (you select the name) with one worksheet labeled "Points." All of your data are listed in this this worksheet. If this worksheet is blank, check the following:

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

Match

Search in: C:\Documents and Settings\Lesley\My Documents\Research\Faience\Faienc

Start energy: 5.8 keV End energy: 6.2 keV

Min. correlation: 50 % Number of hits: 100

Start Cancel Help

Nuzi1450BCFritFaiSpacer_bead_40KV_Obsid-filter_ltblmatrix@221110_091052

File Measurement Analyze Spectrum Project Options Device Export User ?

Nuzi1450BCFritFaiSpacer_bead_40KV_Obsid-filt lg Live Time: 200 s Faience

Nuzi_40kV.rtx Spectrum Parameter Results Match Results Project Scan

Spectrum: Nuzi1450BCFritFaiSpacer_bead_40KV_Obsid-filter_ltblmatrix@221110

Search in: C:\Documents and Settings\Lesley\My Documents\Research\Faience

Start energy: 5.8 keV End energy: 6.2 keV

Min. correlation: 50 % Number of hits: 100

The Match results show up in a new tab

	Correlation/%	Spectrum	Date	Filename
1	100.00	Nuzi1450BCFritFaiSpacer	11/22/2010 9:10:42 AM	C:\Documents and Settings\Lesley\My Documents\Research\Faience\Faience
2	81.35	Nuzi1450BCFaienceMelo	11/22/2010 9:10:41 AM	C:\Documents and Settings\Lesley\My Documents\Research\Faience\Faience
3	79.21	Nuzi1450BCFai-LargeOva	11/22/2010 9:10:41 AM	C:\Documents and Settings\Lesley\My Documents\Research\Faience\Faience
4	55.68	Nuzi1450BCFaienceMelo	11/22/2010 9:10:41 AM	C:\Documents and Settings\Lesley\My Documents\Research\Faience\Faience
5	53.86	Nuzi1450BCGlassyFai-Tu	11/22/2010 9:10:41 AM	C:\Documents and Settings\Lesley\My Documents\Research\Faience\Faience
6	53.54	Nuzi1450BCFaienceMelo	11/22/2010 9:10:41 AM	C:\Documents and Settings\Lesley\My Documents\Research\Faience\Faience

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 $K\alpha$ and $K\beta$ are important!)