030.0101.03.0

S1 TITAN/TRACER 5/CTX

EasyCal— A Comic Strip

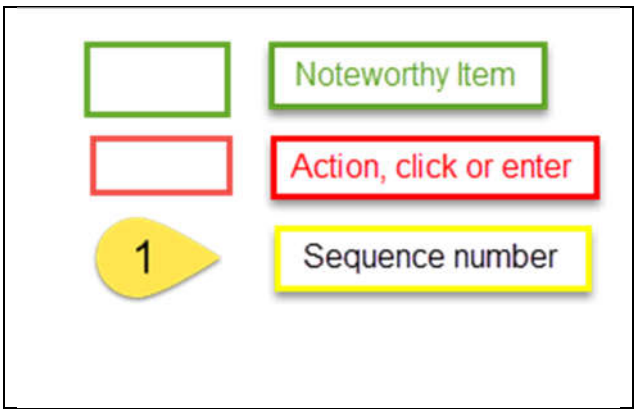
V.2.5.61

Handheld XRF

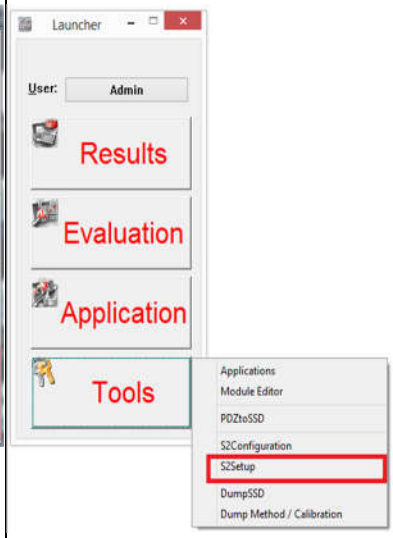
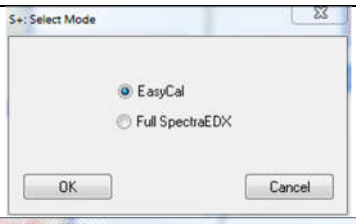
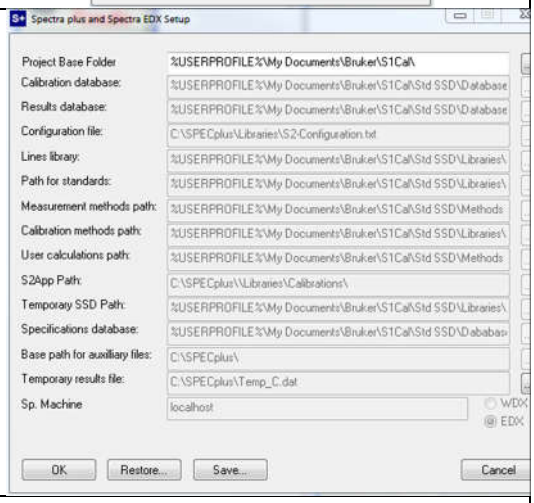
Innovation with Integrity

A COMIC STRIP

Contents


Noteworthy Item
Action, click or enter
1
Sequence number

1 Setting up the Workspace.

EasyCal Launcher			S2Setup
Double Click			 
			See Appendix A for more information about “Project Base Folder”

2. A New Calibration.

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<tr>
<td> 
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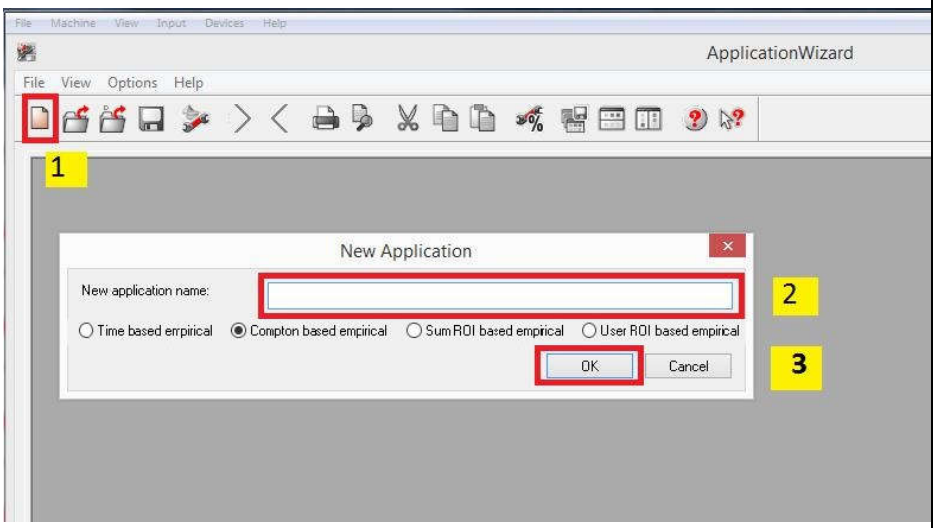
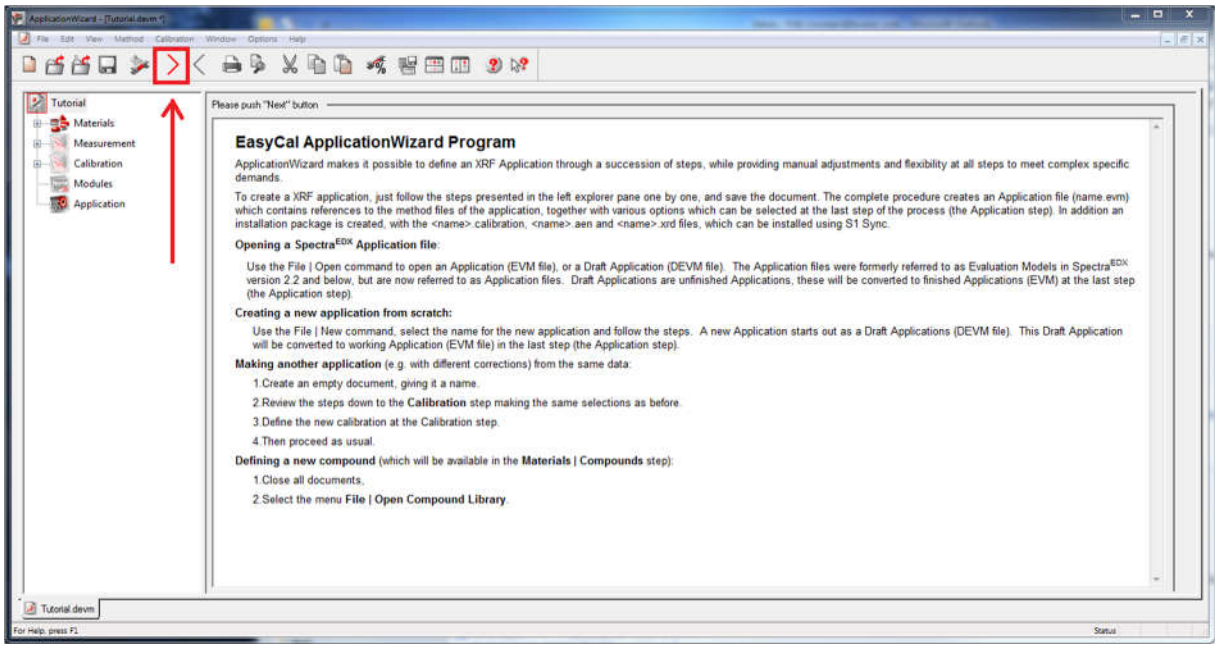
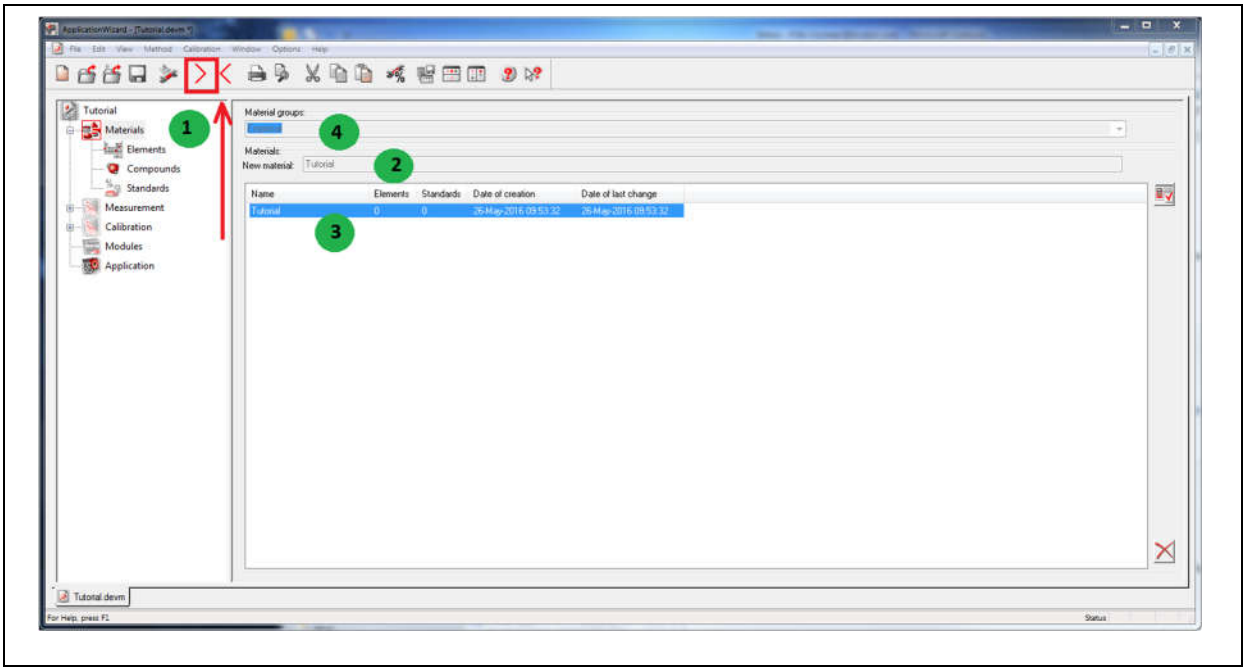
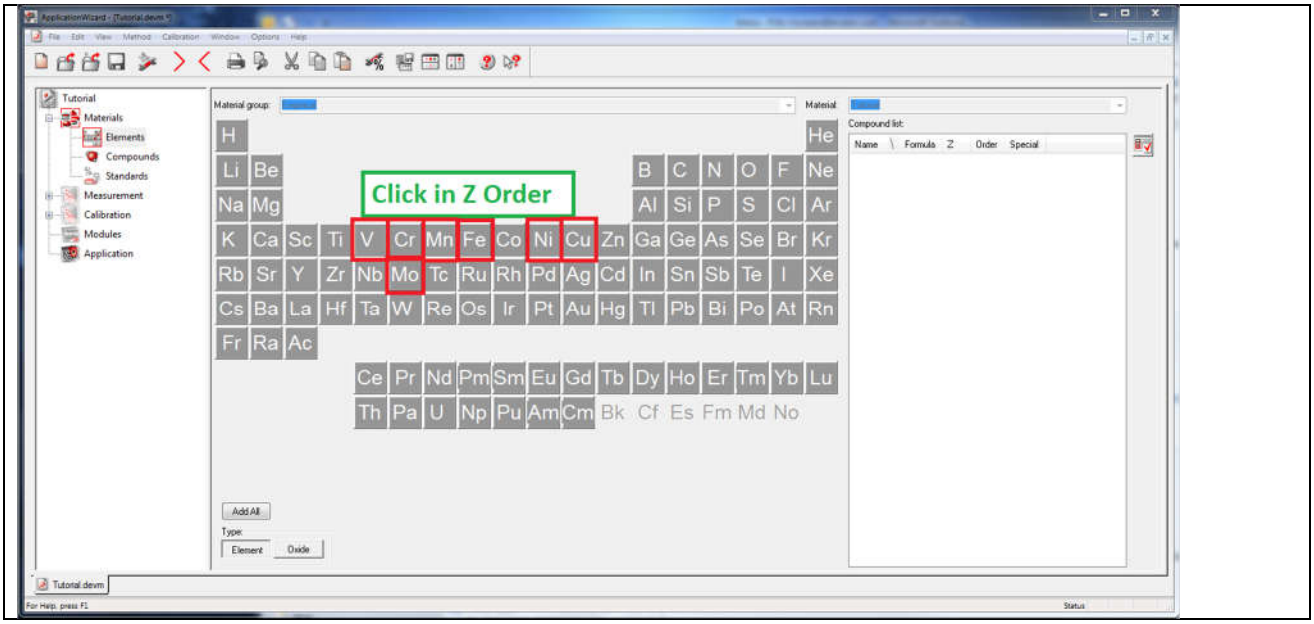
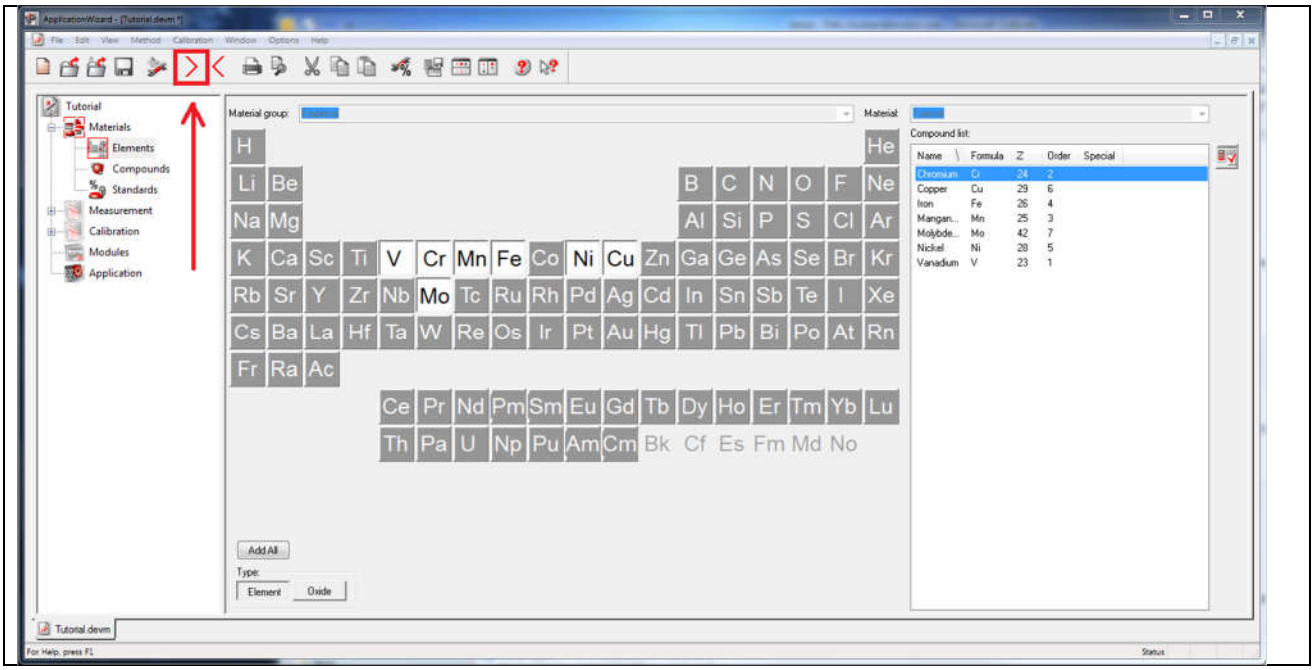
<td> 
</td>
</tr>
<tr>
<td>Note</td>
<td>The internal standard selected when creating a new calibration will be used as the default for each element as they are added to the calibration. The active internal standard can be changed on an element by element basis at a later point in the process. The default selected at this point cannot be changed.</td>
</tr>
</table>



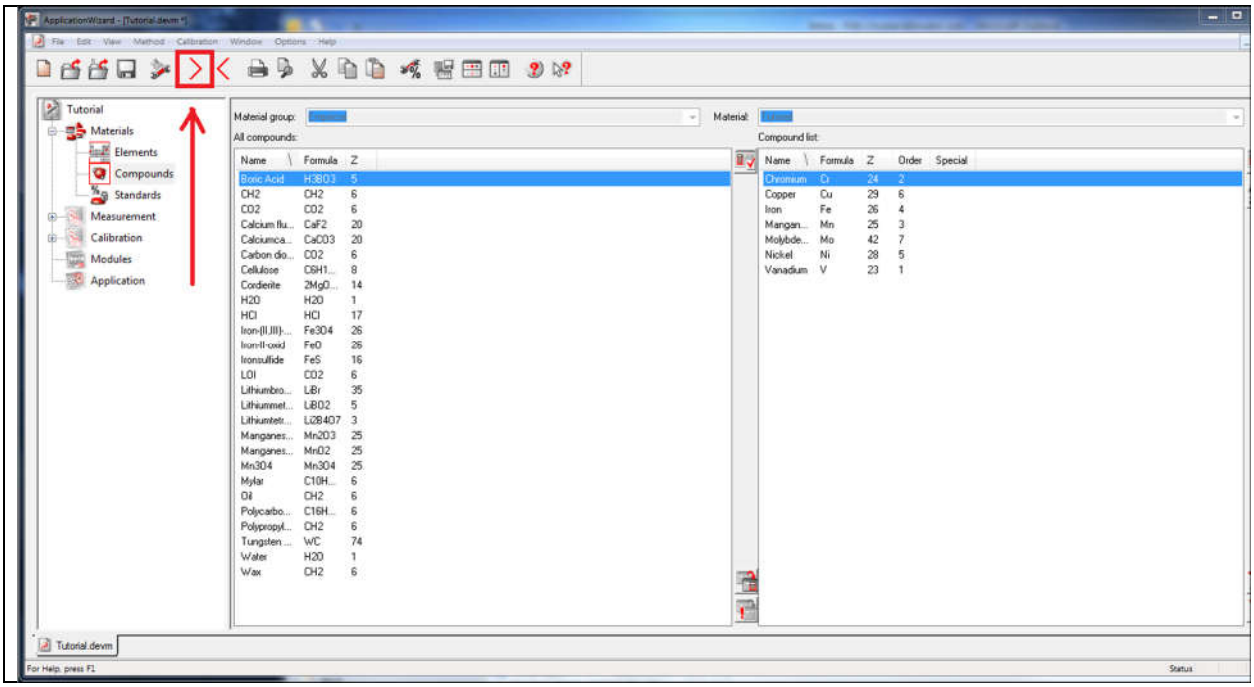


2.1 Select the elements.

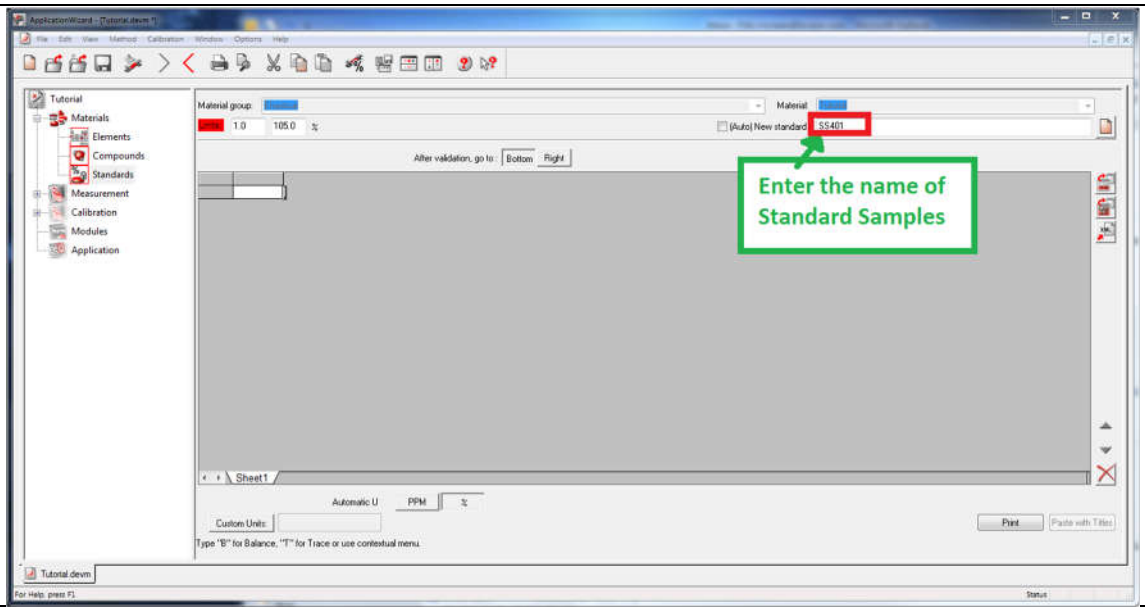


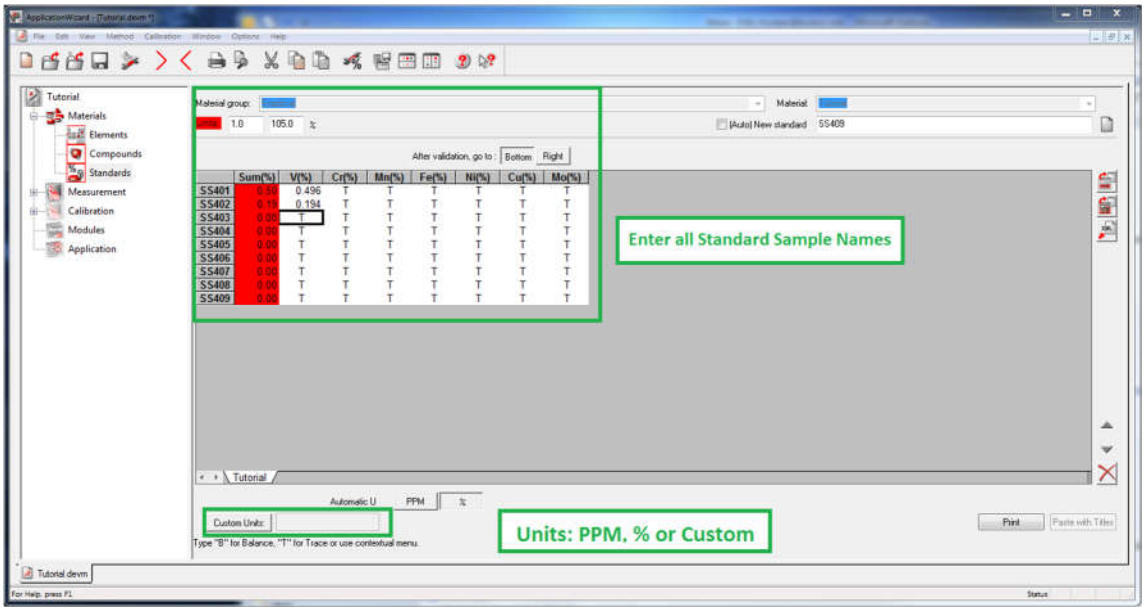

Tutorial
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material group:
Material:
Compound list:
Name
Formula
Z
Order
Special
Chromium Cr 24 2
Copper Cu 29 6
Iron Fe 26 4
Mangan... Mn 25 3
Molybde... Mo 42 7
Nickel Ni 28 5
Vanadium V 23 1
Add All
Type:
Element
Oxide
Tutorial.devm

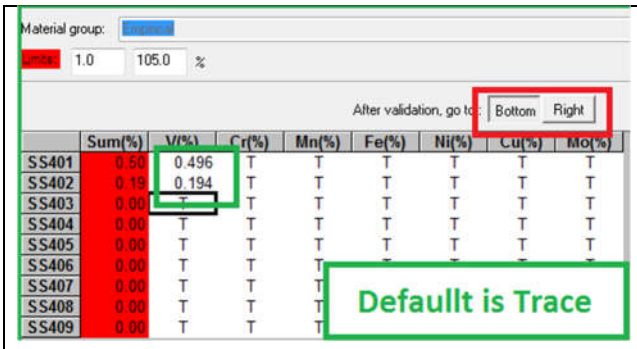
2.2 Adding Compounds.

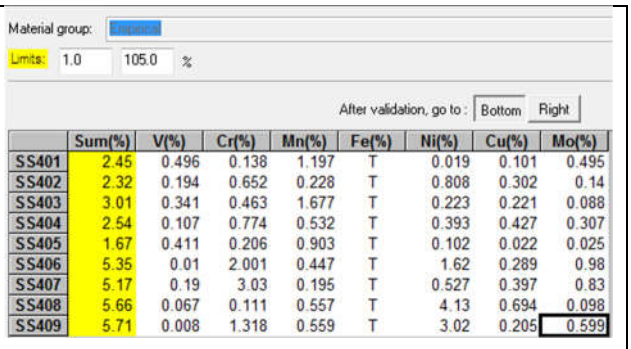


2.3 Enter Standard Sample Names and Concentrations.

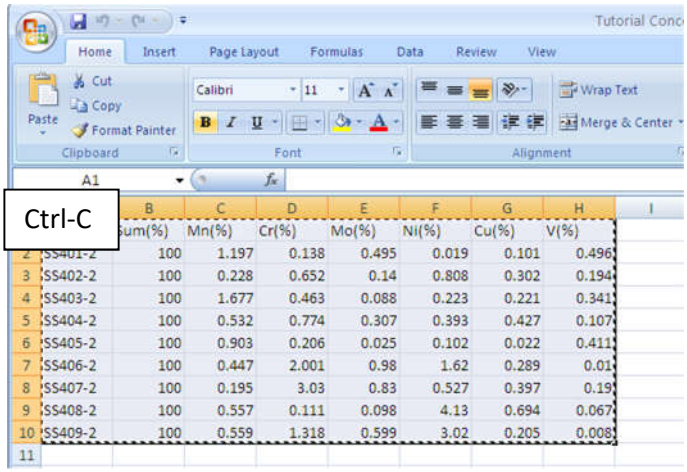




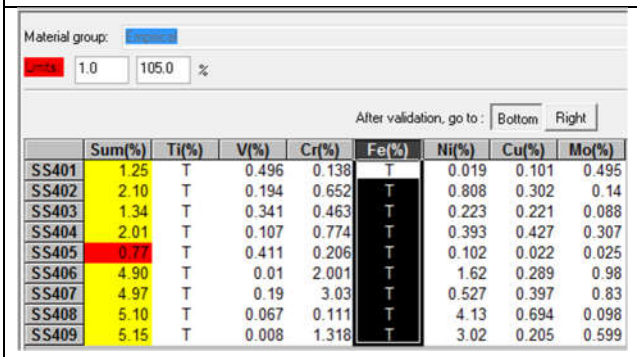

Material group:
Limits: 1.0 105.0 %
After validation, go to: Bottom Right
Defaullt is Trace

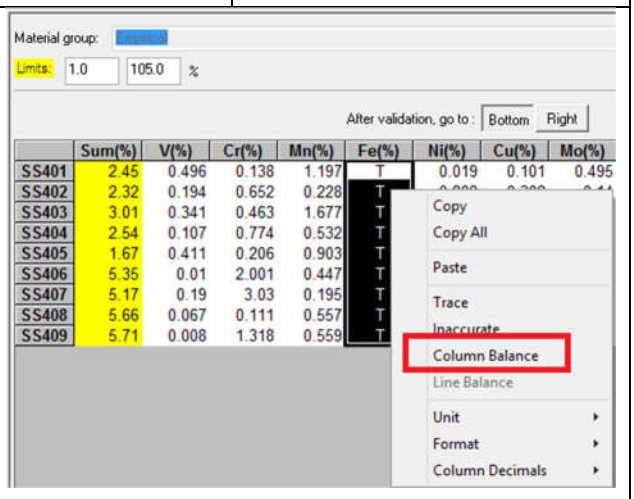

Material group:
Limits: 1.0 105.0 %
After validation, go to: Bottom Right

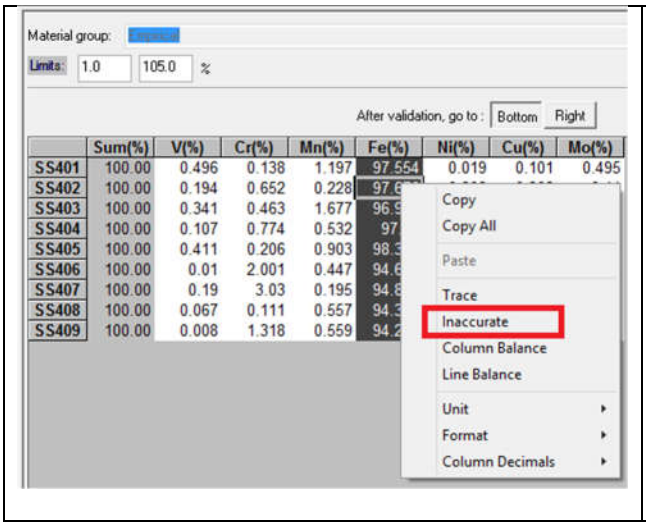
-OR-

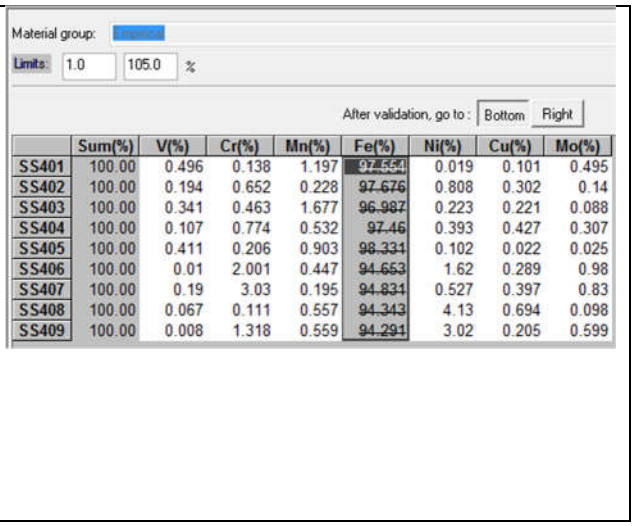

Ctrl-C

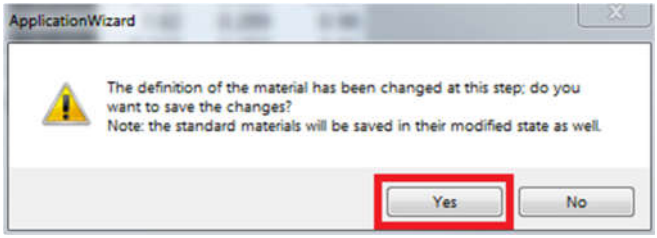

Paste with Titles


Material group:
Limits: 1.0 105.0 %
After validation, go to: Bottom Right


Material group:
Limits: 1.0 105.0 %
After validation, go to: Bottom Right
Copy
Copy All
Paste
Trace
Inaccurate
Column Balance
Line Balance
Unit
Format
Column Decimals

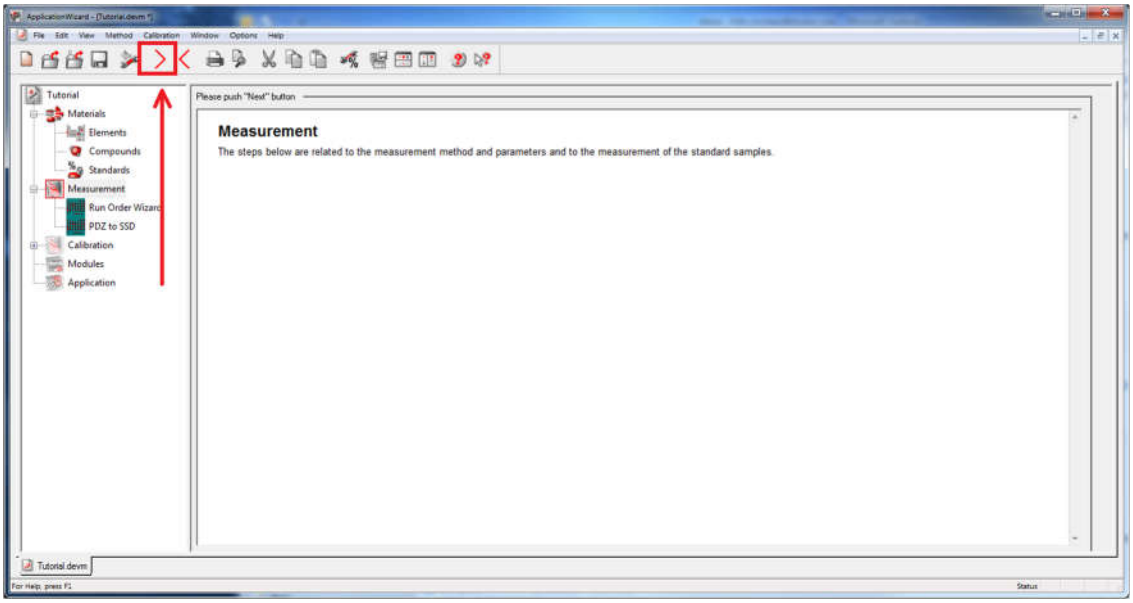

Material group:
Limits: 1.0 105.0 %
After validation, go to : Bottom Right
Sum(%) V(%) Cr(%) Mn(%) Fe(%) Ni(%) Cu(%) Mo(%)
SS401 100.00 0.496 0.138 1.197 97.554 0.019 0.101 0.495
SS402 100.00 0.194 0.652 0.228 97.6
SS403 100.00 0.341 0.463 1.677 96.9
SS404 100.00 0.107 0.774 0.532 97
SS405 100.00 0.411 0.206 0.903 98.3
SS406 100.00 0.01 2.001 0.447 94.6
SS407 100.00 0.19 3.03 0.195 94.8
SS408 100.00 0.067 0.111 0.557 94.3
SS409 100.00 0.008 1.318 0.559 94.2
Copy
Copy All
Paste
Trace
Inaccurate
Column Balance
Line Balance
Unit
Format
Column Decimals

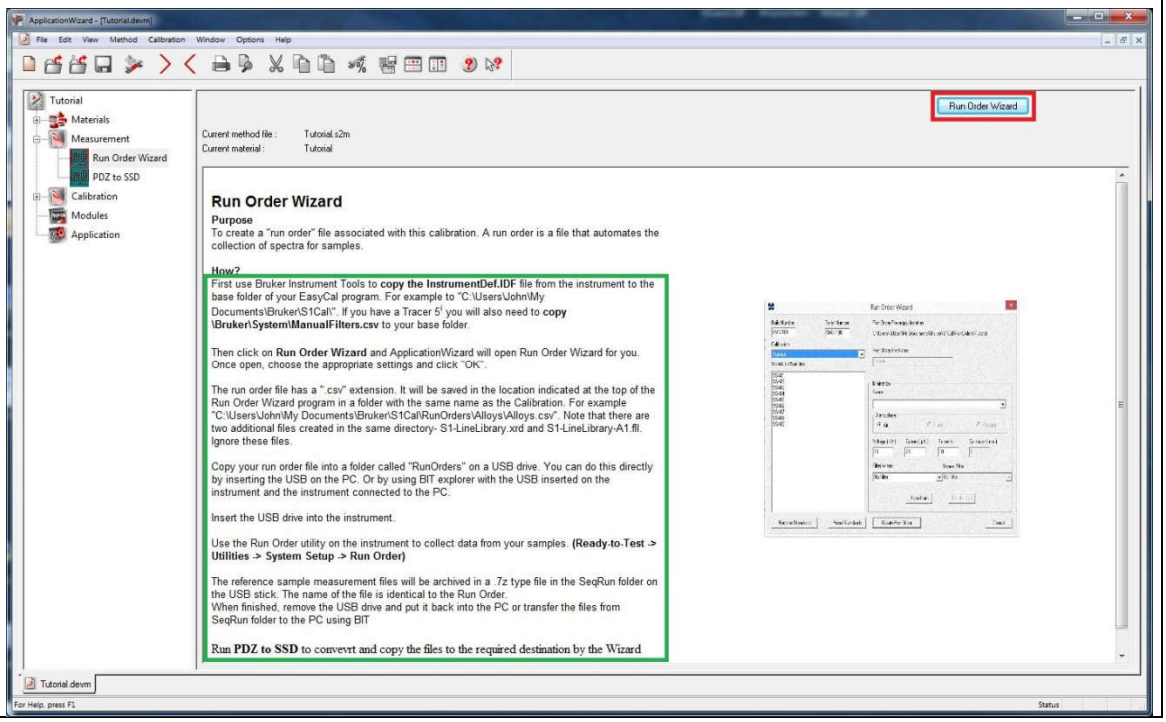

Material group:
Limits: 1.0 105.0 %
After validation, go to : Bottom Right
Sum(%) V(%) Cr(%) Mn(%) Fe(%) Ni(%) Cu(%) Mo(%)
SS401 100.00 0.496 0.138 1.197 97.554 0.019 0.101 0.495
SS402 100.00 0.194 0.652 0.228 97.676 0.808 0.302 0.14
SS403 100.00 0.341 0.463 1.677 96.987 0.223 0.221 0.088
SS404 100.00 0.107 0.774 0.532 97.46 0.393 0.427 0.307
SS405 100.00 0.411 0.206 0.903 98.331 0.102 0.022 0.025
SS406 100.00 0.01 2.001 0.447 94.653 1.62 0.289 0.98
SS407 100.00 0.19 3.03 0.195 94.831 0.527 0.397 0.83
SS408 100.00 0.067 0.111 0.557 94.343 4.13 0.694 0.098
SS409 100.00 0.008 1.318 0.559 94.291 3.02 0.205 0.599

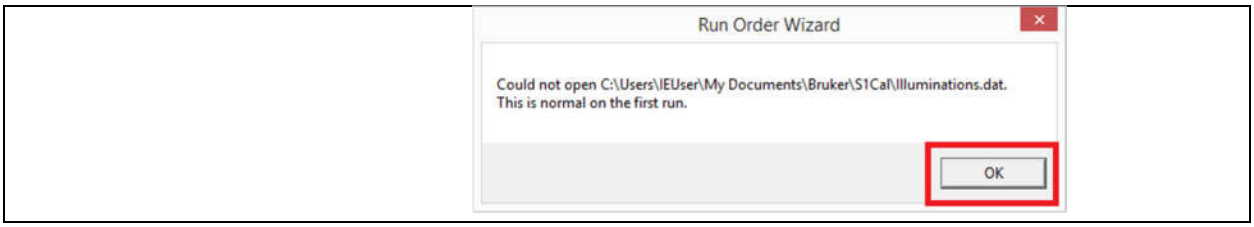

ApplicationWizard
The definition of the material has been changed at this step; do you want to save the changes?
Note: the standard materials will be saved in their modified state as well.
Yes
No

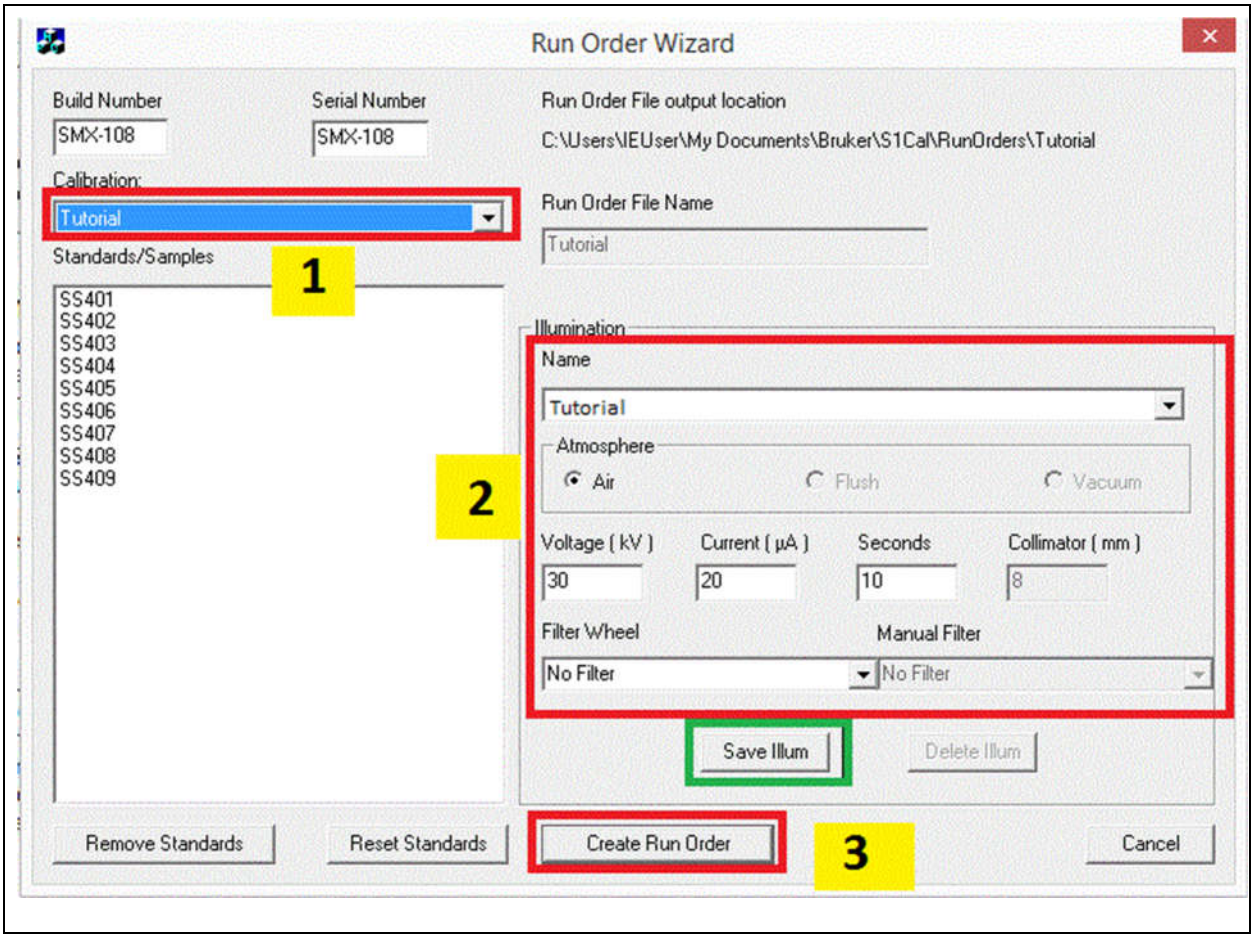
3 Measuring the Assays.

3.1 Creating the Run Order.

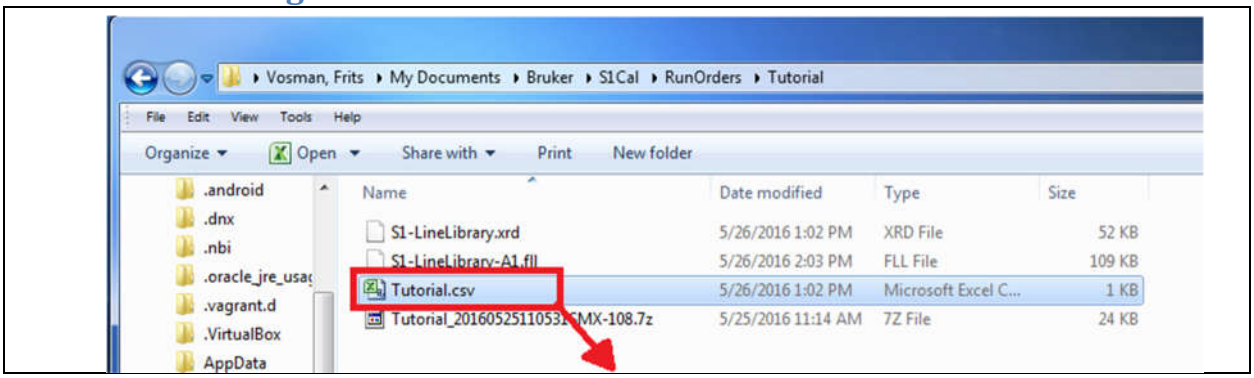


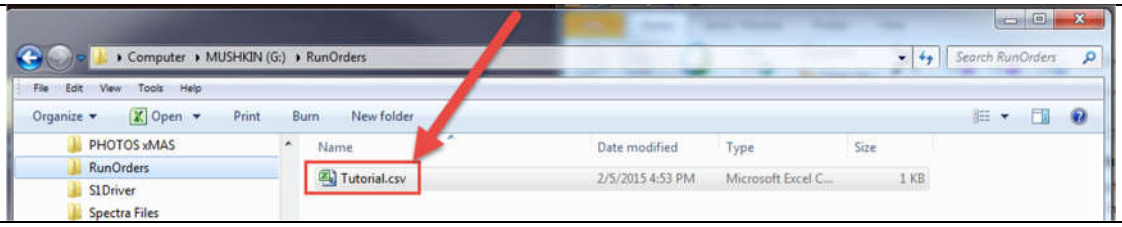




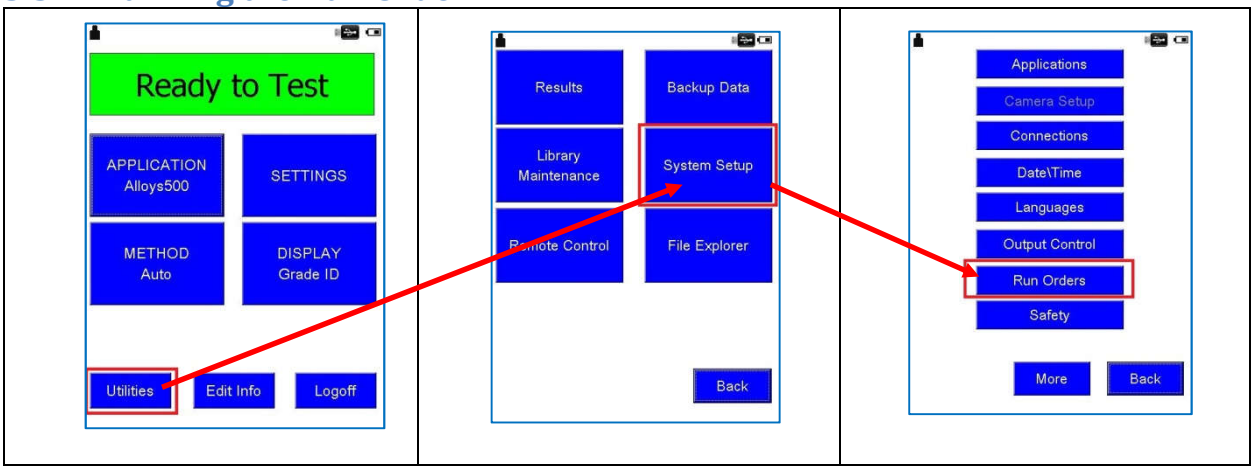


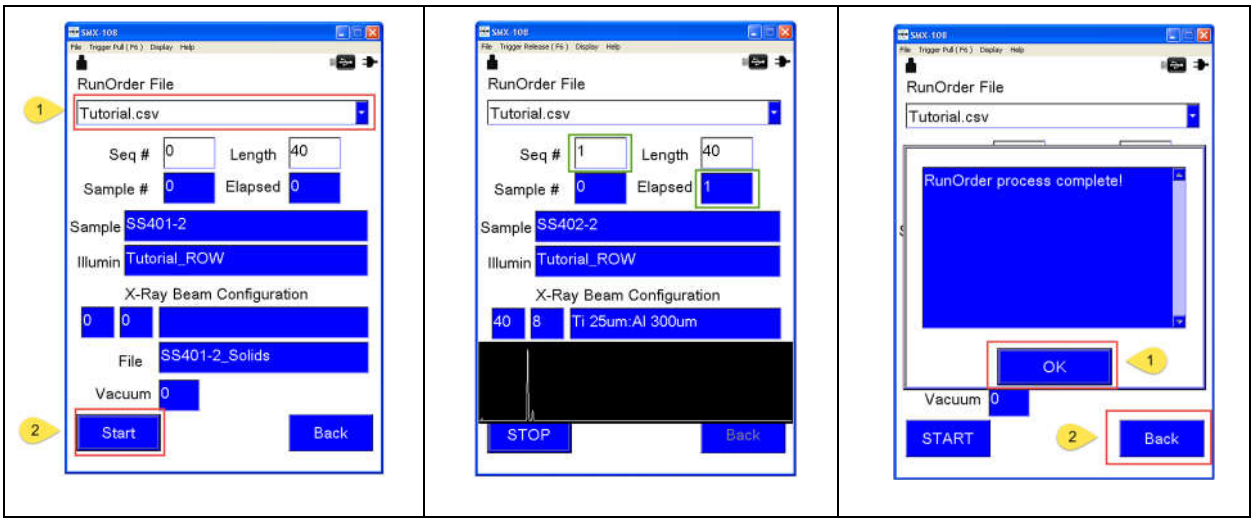
3.2 Transferring the Run Order to the Instrument.



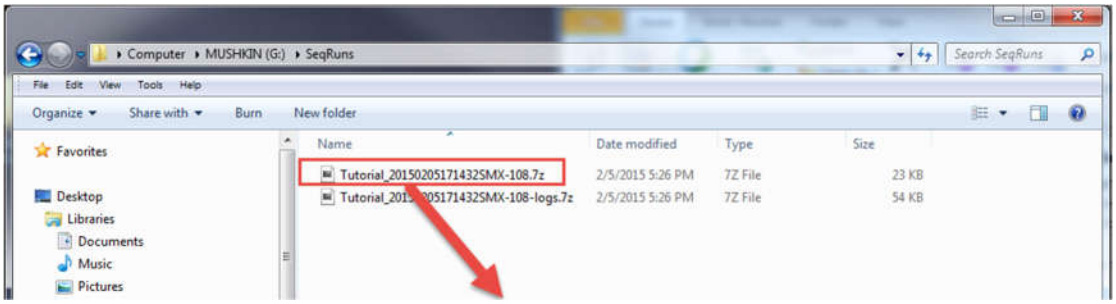
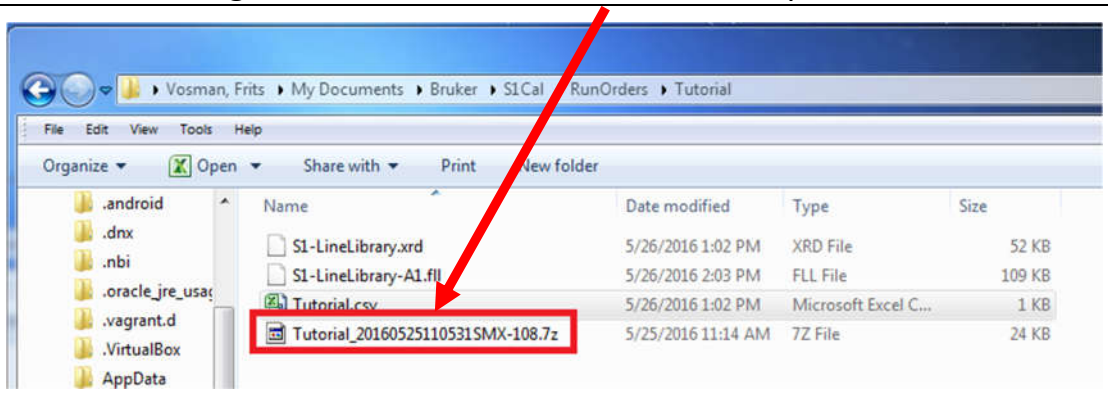
Drag csv file to USB stick into RunOrders folder

Move USB stick to the intstrument

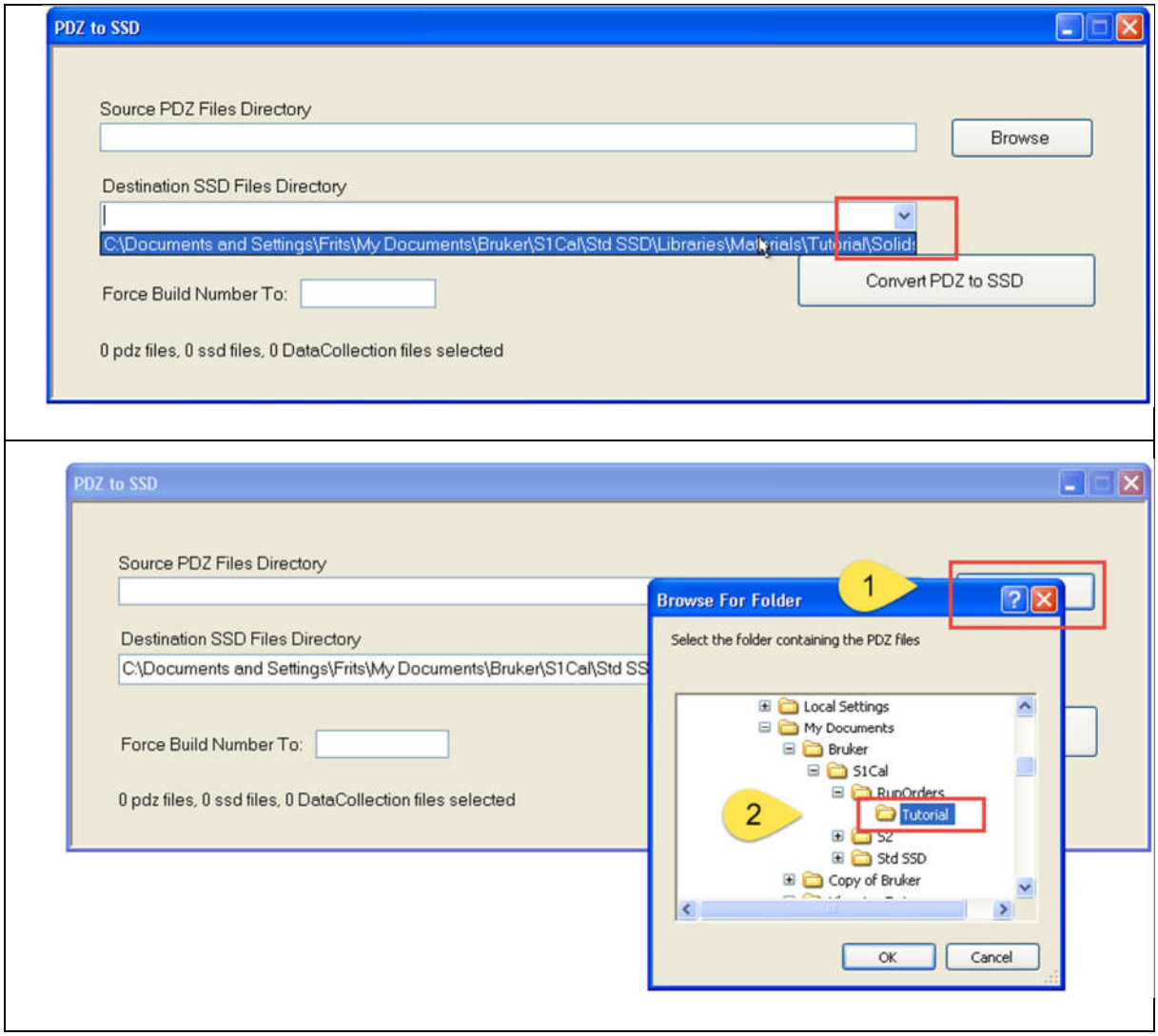
3.3 Running the Run Order.

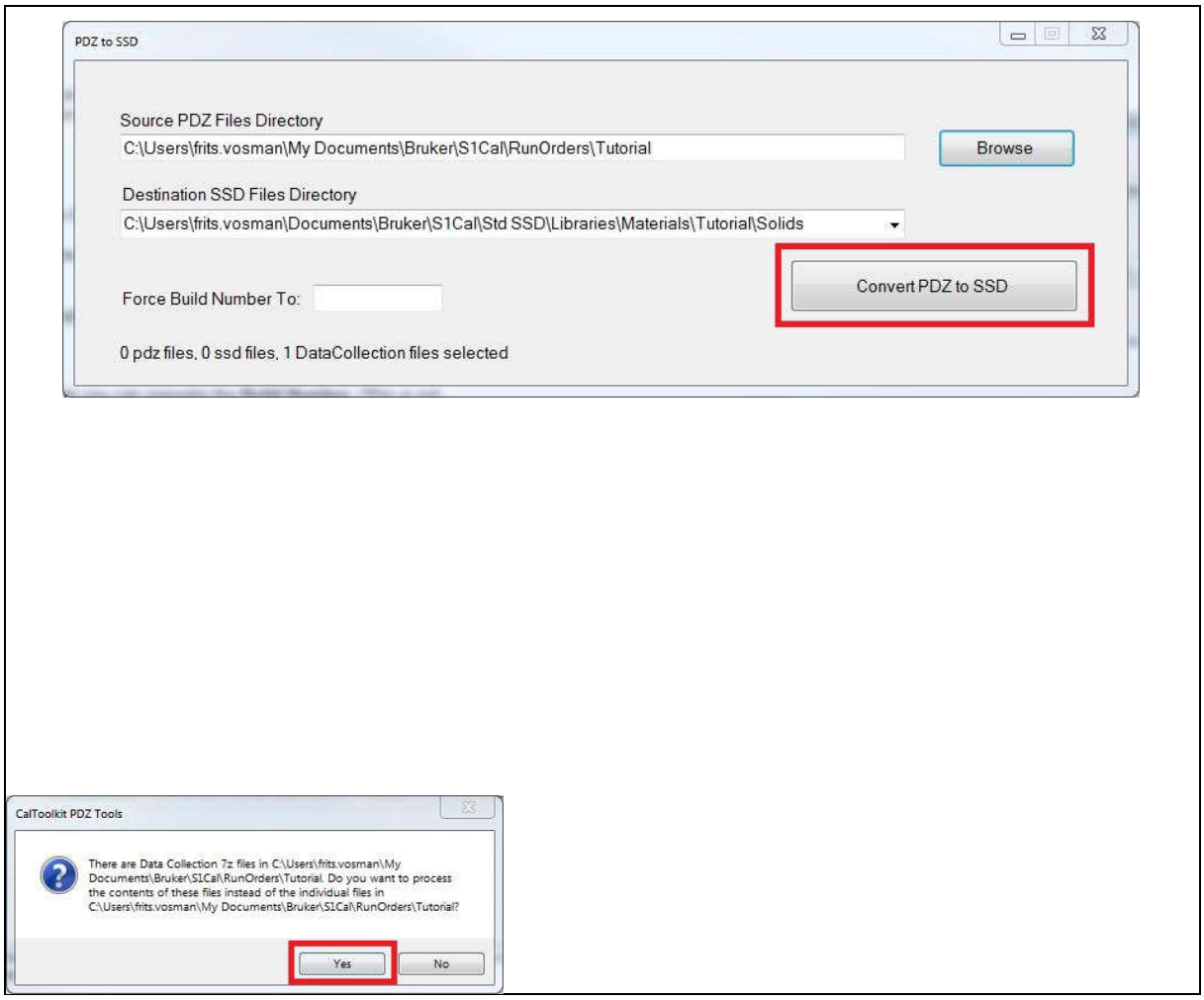


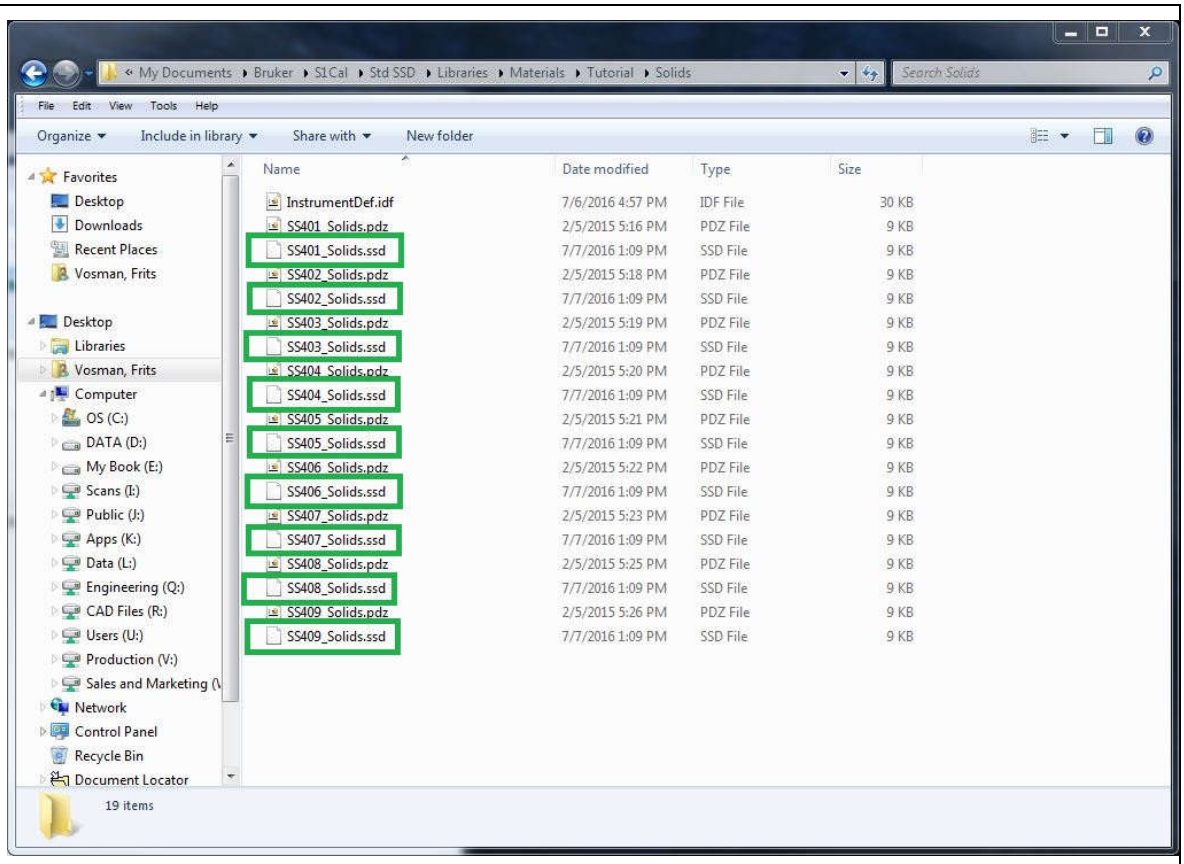


3.4 Transferring the Data to the PC.

Move USB stick to computer

Drag the 7z file from the USB to the computer.



PDZ to SSD
Source PDZ Files Directory
Browse
Destination SSD Files Directory
C:\Documents and Settings\Frits\My Documents\Bruker\S1Cal\Std SSD\Libraries\Materials\Tutorial\Solids
Force Build Number To:
Convert PDZ to SSD
0 pdz files, 0 ssd files, 0 DataCollection files selected
PDZ to SSD
Source PDZ Files Directory
Destination SSD Files Directory
C:\Documents and Settings\Frits\My Documents\Bruker\S1Cal\Std SS
Force Build Number To:
0 pdz files, 0 ssd files, 0 DataCollection files selected
Browse For Folder
1
Select the folder containing the PDZ files
Local Settings
My Documents
Bruker
S1Cal
RunOrders
2
Tutorial
S2
Std SSD
Copy of Bruker
OK
Cancel


PDZ to SSD
Source PDZ Files Directory
C:\Users\frits.vosman\My Documents\Bruker\S1Cal\RunOrders\Tutorial
Browse
Destination SSD Files Directory
C:\Users\frits.vosman\Documents\Bruker\S1Cal\Std SSD\Libraries\Materials\Tutorial\Solids
Force Build Number To:
Convert PDZ to SSD
0 pdz files, 0 ssd files, 1 DataCollection files selected
CalToolkit PDZ Tools
There are Data Collection 7z files in C:\Users\frits.vosman\My Documents\Bruker\S1Cal\RunOrders\Tutorial. Do you want to process the contents of these files instead of the individual files in C:\Users\frits.vosman\My Documents\Bruker\S1Cal\RunOrders\Tutorial?
Yes
No


My Documents ▸ Bruker ▸ S1Cal ▸ Std SSD ▸ Libraries ▸ Materials ▸ Tutorial ▸ Solids
Search Solids
File Edit View Tools Help
Organize Include in library Share with New folder
Favorites
Desktop
Downloads
Recent Places
Vosman, Frits
Desktop
Libraries
Vosman, Frits
Computer
OS (C:)
DATA (D:)
My Book (E:)
Scans (I:)
Public (J:)
Apps (K:)
Data (L:)
Engineering (Q:)
CAD Files (R:)
Users (U:)
Production (V:)
Sales and Marketing (\
Network
Control Panel
Recycle Bin
Document Locator
19 items
Name
Date modified
Type
Size
InstrumentDef.idf 7/6/2016 4:57 PM IDF File 30 KB
SS401_Solids.pdz 2/5/2015 5:16 PM PDZ File 9 KB
SS401_Solids.ssd 7/7/2016 1:09 PM SSD File 9 KB
SS402_Solids.pdz 2/5/2015 5:18 PM PDZ File 9 KB
SS402_Solids.ssd 7/7/2016 1:09 PM SSD File 9 KB
SS403_Solids.pdz 2/5/2015 5:19 PM PDZ File 9 KB
SS403_Solids.ssd 7/7/2016 1:09 PM SSD File 9 KB
SS404_Solids.pdz 2/5/2015 5:20 PM PDZ File 9 KB
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SS405_Solids.pdz 2/5/2015 5:21 PM PDZ File 9 KB
SS405_Solids.ssd 7/7/2016 1:09 PM SSD File 9 KB
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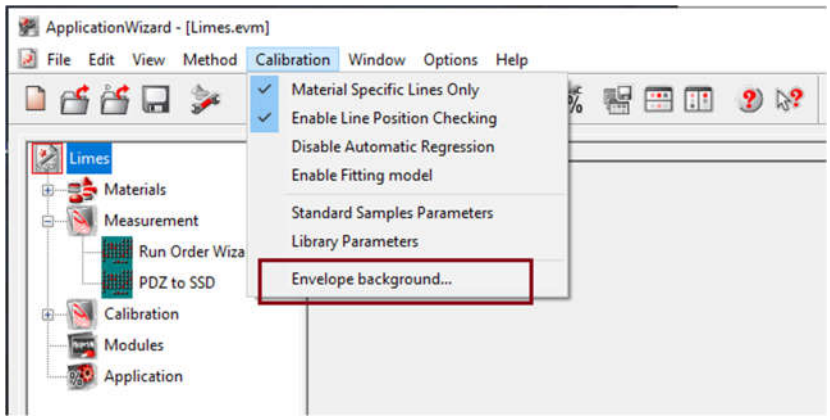
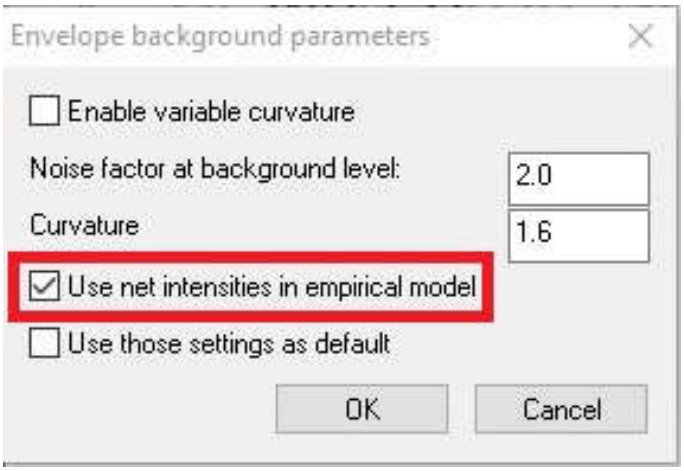
SS406_Solids.ssd 7/7/2016 1:09 PM SSD File 9 KB
SS407_Solids.pdz 2/5/2015 5:23 PM PDZ File 9 KB
SS407_Solids.ssd 7/7/2016 1:09 PM SSD File 9 KB
SS408_Solids.pdz 2/5/2015 5:25 PM PDZ File 9 KB
SS408_Solids.ssd 7/7/2016 1:09 PM SSD File 9 KB
SS409_Solids.pdz 2/5/2015 5:26 PM PDZ File 9 KB
SS409_Solids.ssd 7/7/2016 1:09 PM SSD File 9 KB

4. Setting Envelop background subtraction

<table>
<tr>
<td> 
</td>
<td>The Envelope background option found on the Calibration Menu can be used to configure how element peak intensities are calculated. Use of Net intensity, the background under the peak is subtracted, is the default. This behavior can be changed by selecting options from the Envelope background parameters form.</td>
</tr>
<tr>
<td> 
</td>
<td>Uncheck the “Use net intensities in empirical model” check box to use Raw peak intensities.

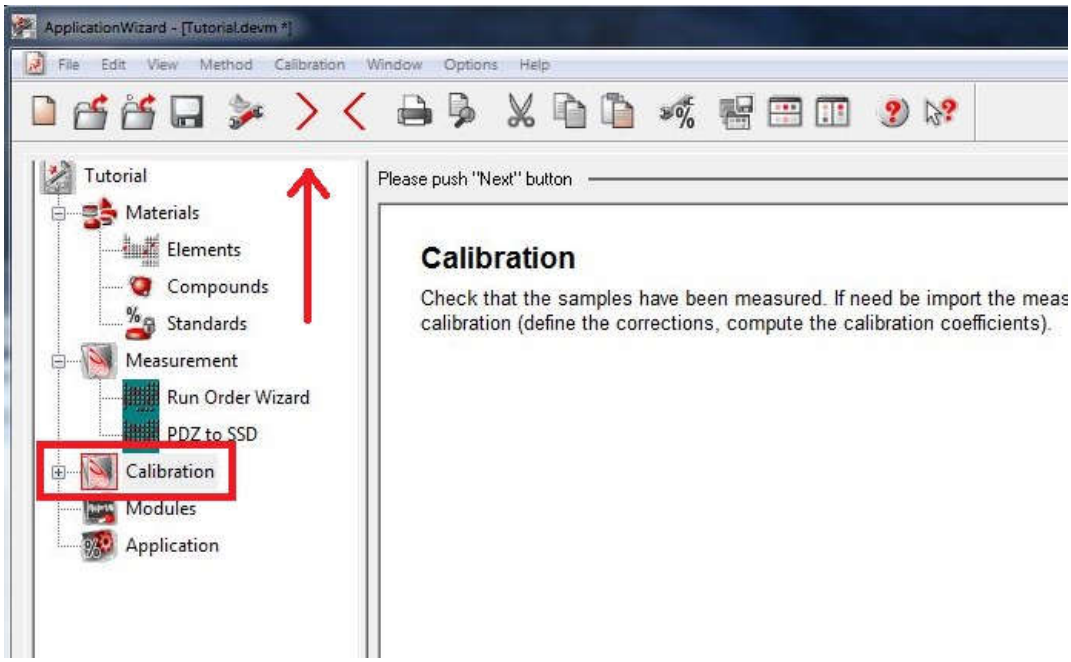
* Checking the “Use those settings as default” box and clicking the “OK” button will cause the entered values to be used as the default for all calibrations created subsequent to this change.

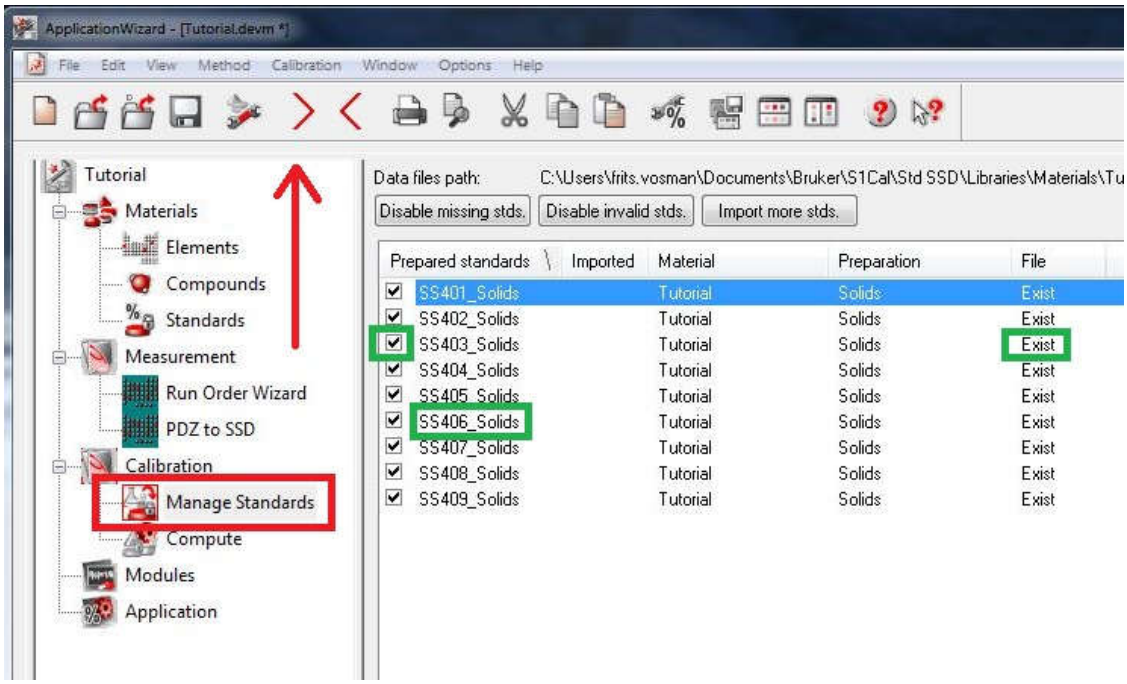
** The other values found on this form should only be changed if the user is an expert with this tool.

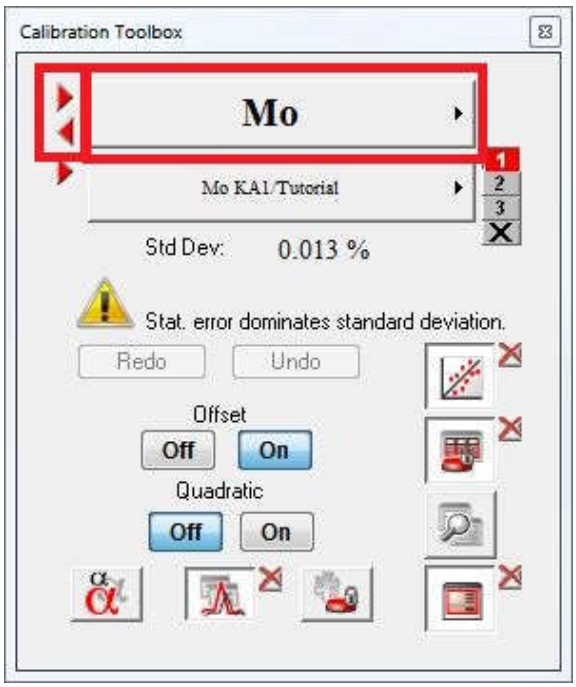
*** CalToolkitEC uses 2.0 and 1.6 as well.</td>
</tr>
</table>

5. Calibration.

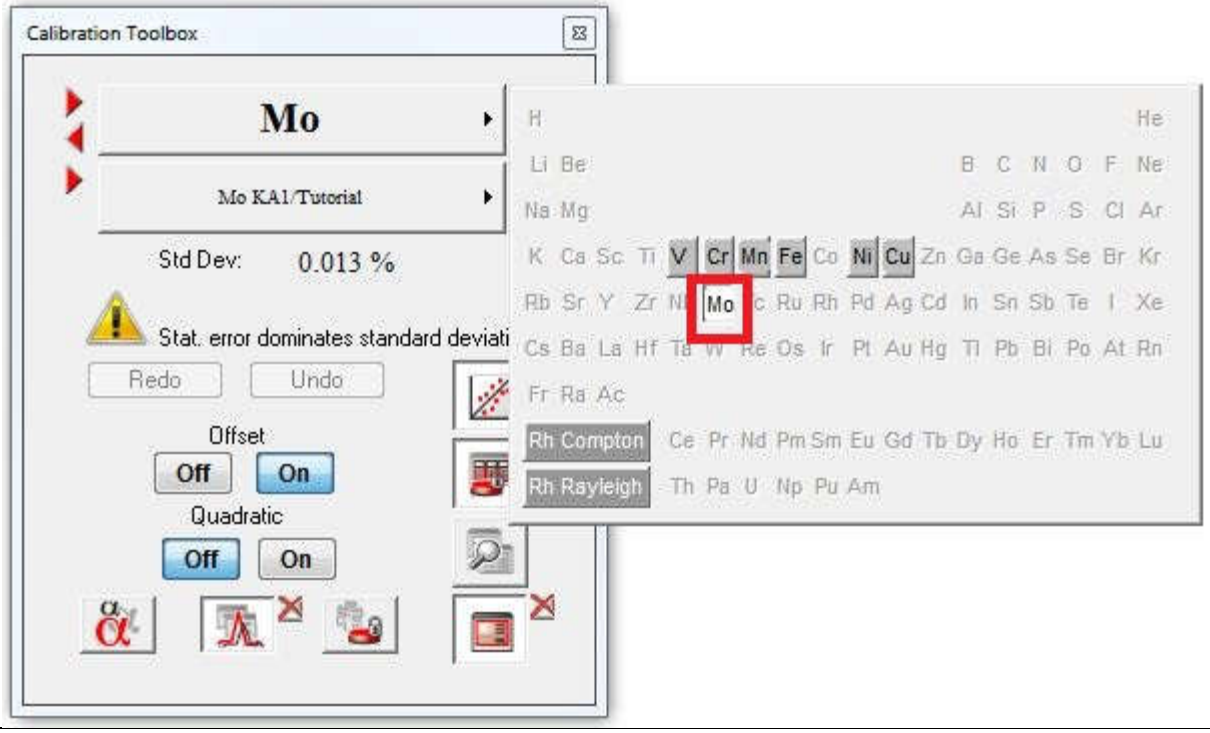
5.1 Importing the data into EasyCal.



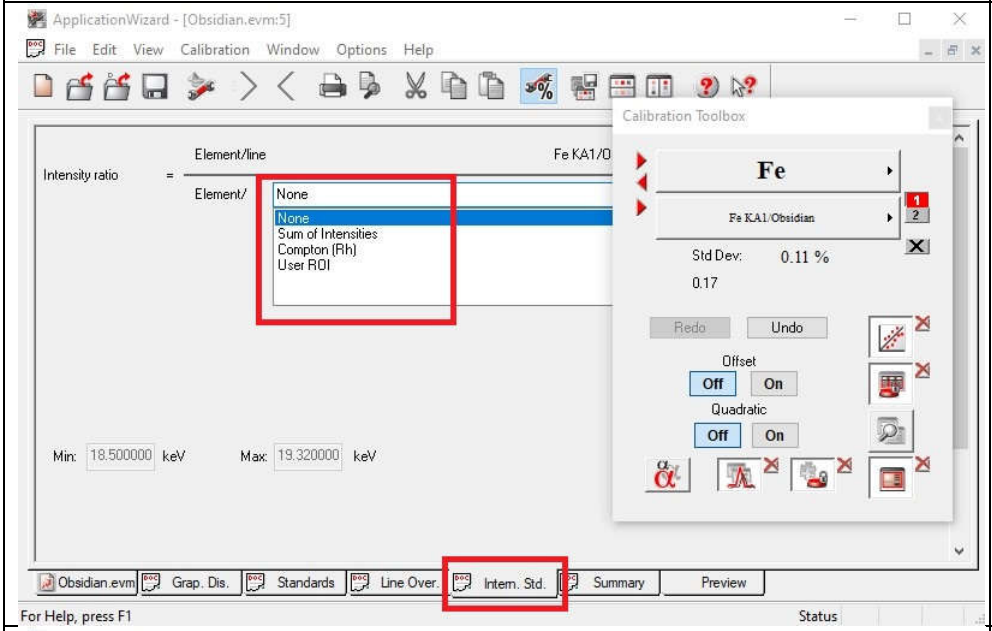




Select the element with the largest Z value. Click on the two left/right arrow buttons to scroll through the elements. Or click on the button with the element, which will bring up the periodic chart.

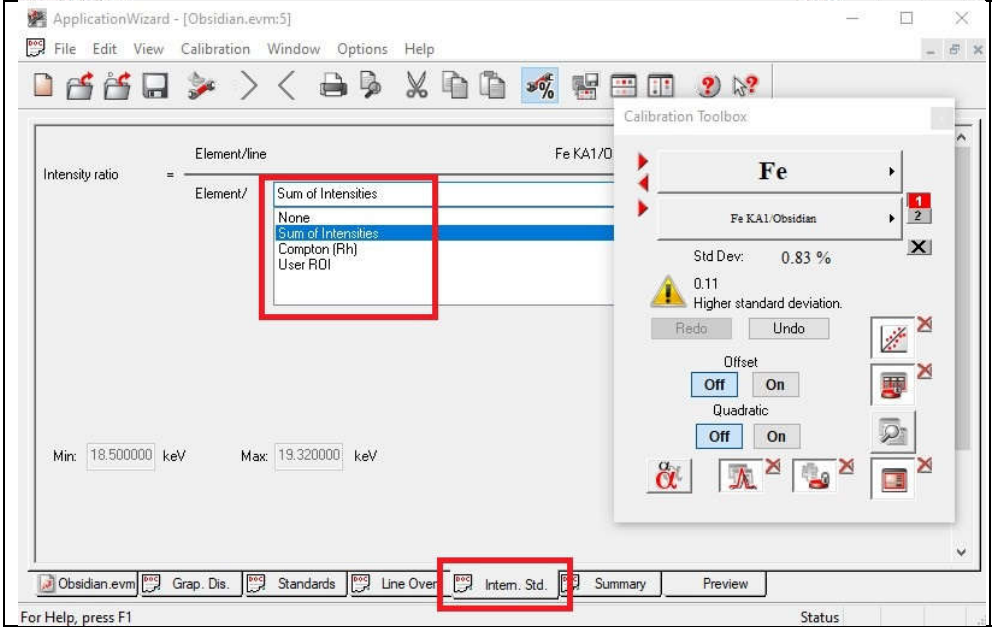


Internal Standards
Note: Each element in the calibration can use a different internal standard.
A single range can be defined for the User ROI option.



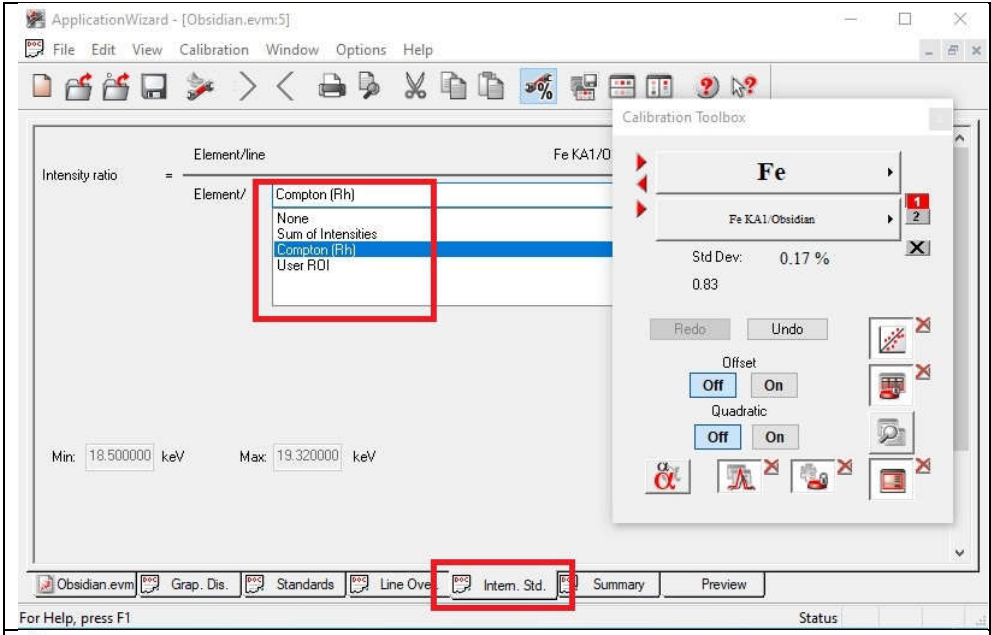
Internal Standard:
None

This selection uses the assay acquisition length to normalize the peak intensity to counts per second.



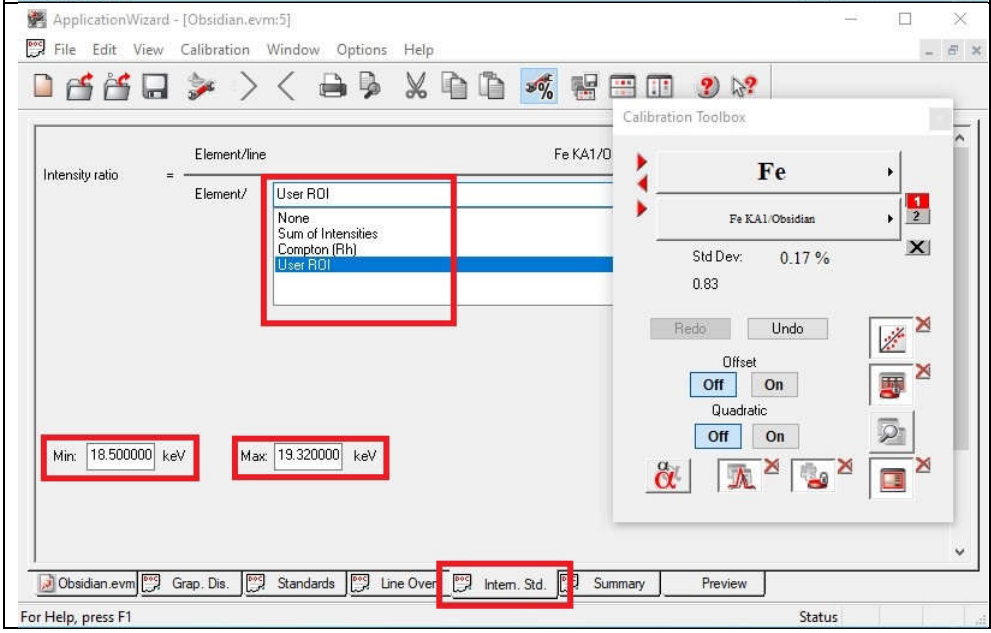
Internal Standard:
Sum of Intensities

This selection uses the accumulated peak intensities of all other elements in the calibration as the normalizing divisor.



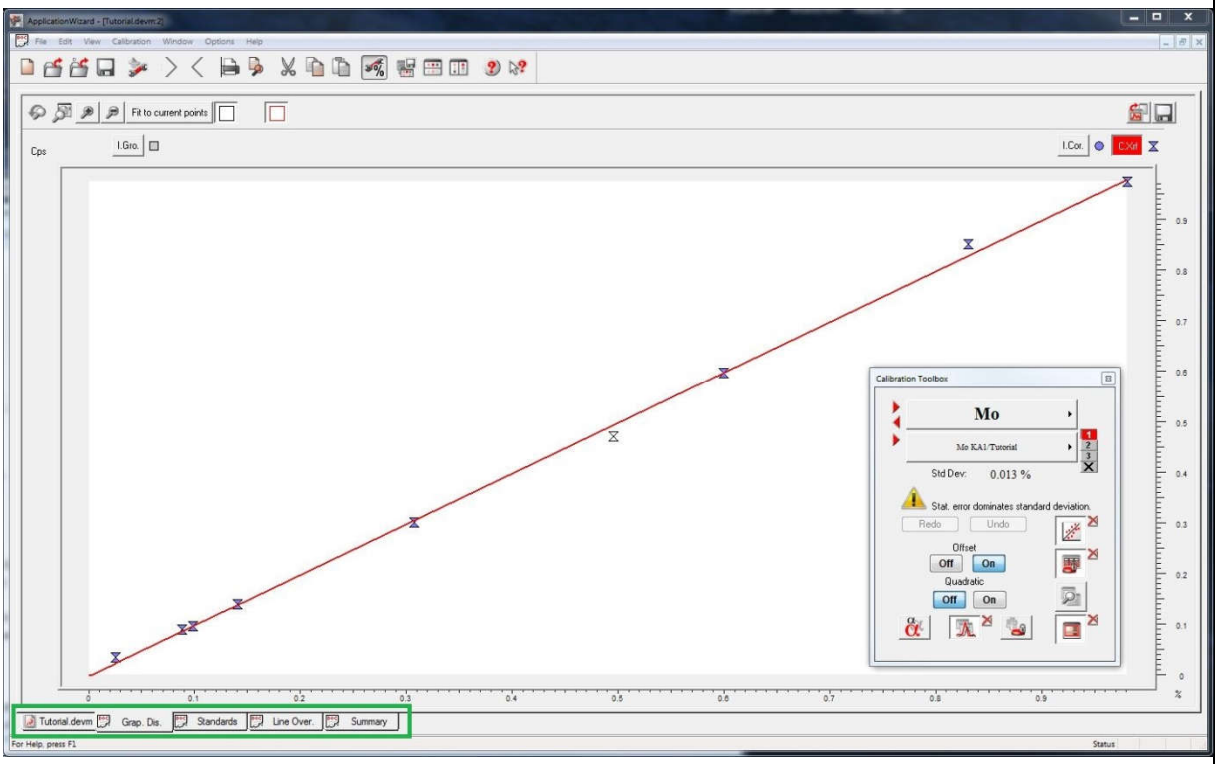
Internal Standard:
Compton (Rh)

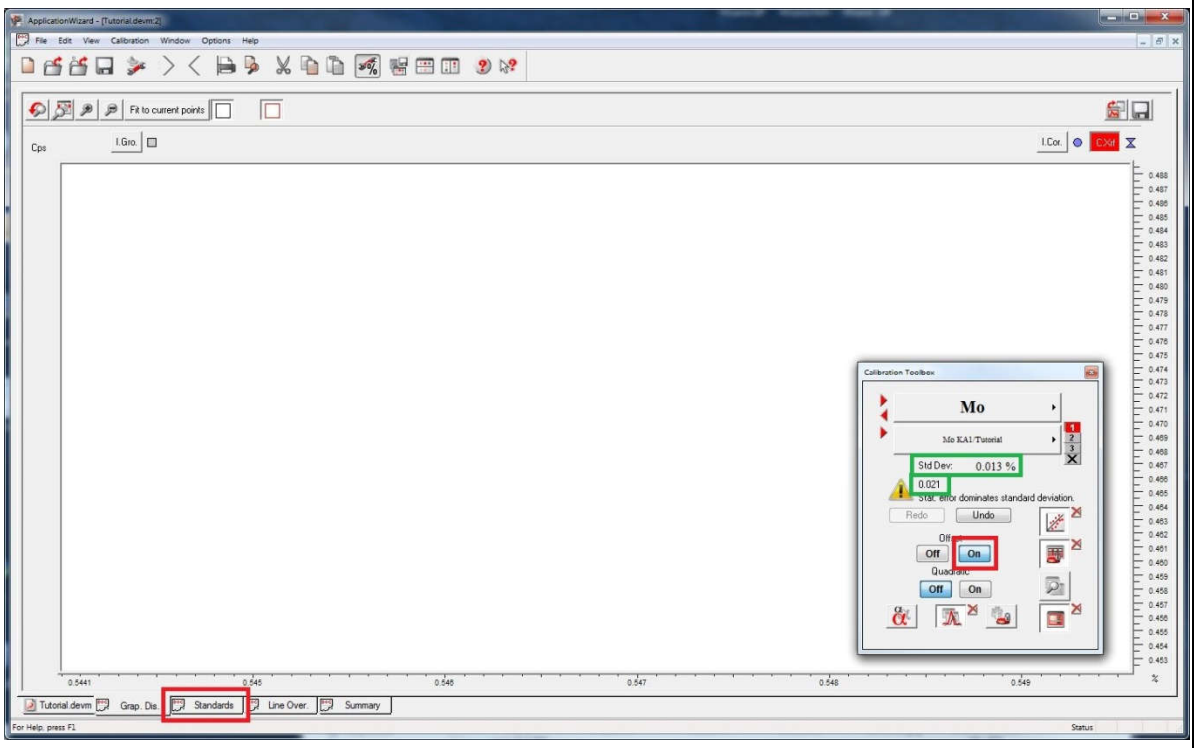
This selection uses the Compton scattering region of the x-ray source target element as the normalizing divisor. Generally this will be the Compton region of the Rh element.

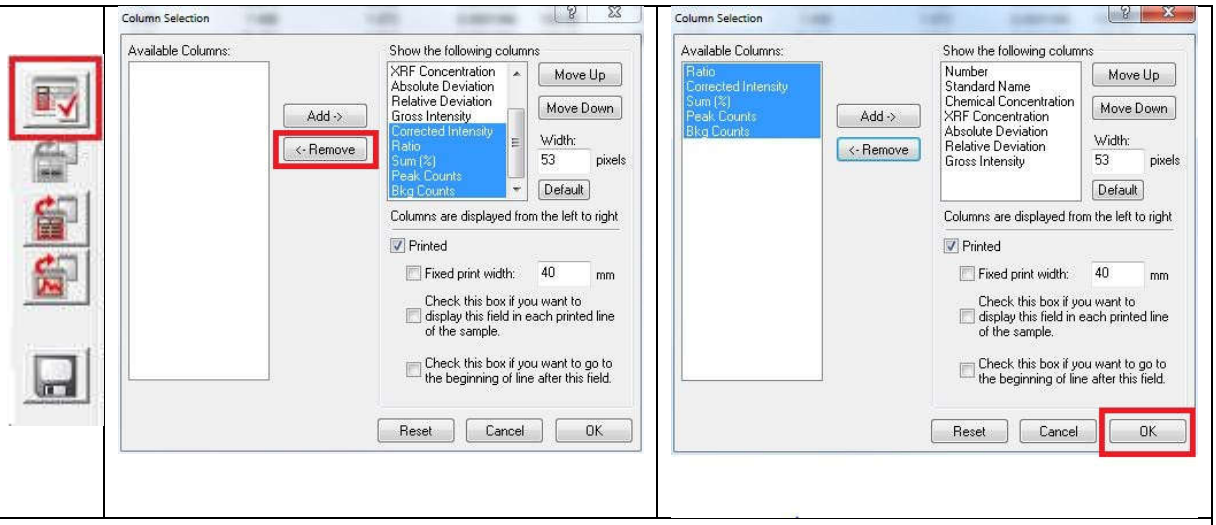


Internal Standard:
User ROI

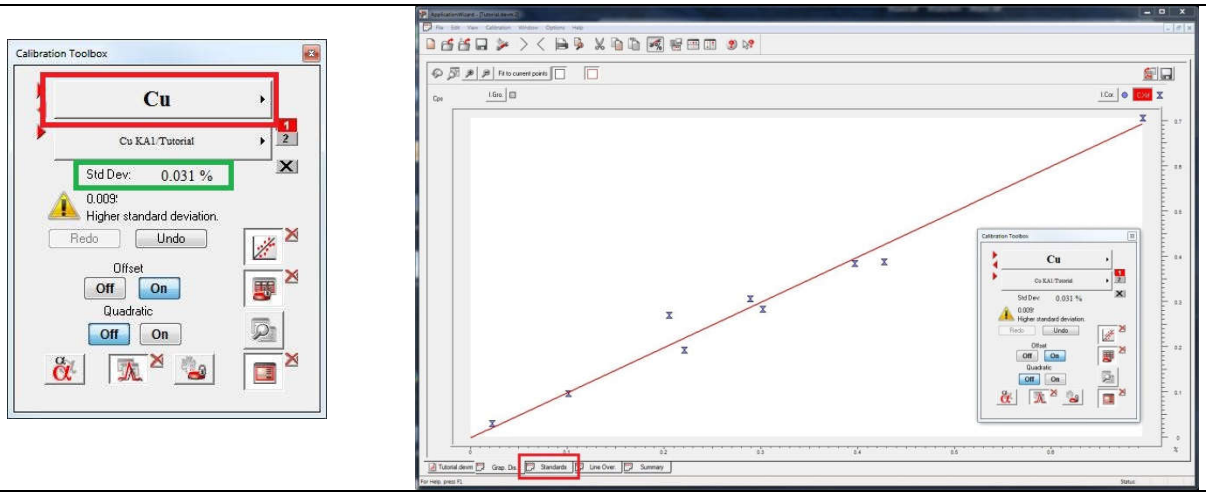
This selection is similar to Compton (Rh) with the exception that the user sets the ROI that's used as the normalizer. The region is defined using the Min and Max fields. The values are entered in keV of energy.


Fit to current points
Cps
I.Gro.
I.Cor.
Calibration Toolbox
Mo
Mo KA1/Tutorial
Std Dev: 0.013 %
Stat. error dominates standard deviation.
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Tutorial.devm
Grap. Dis.
Standards
Line Over.
Summary
For Help, press F1
Status

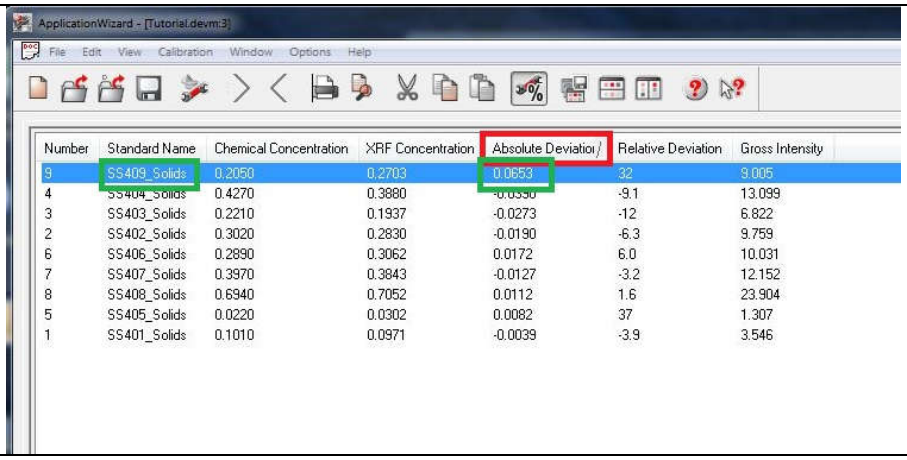

Fit to current points
Cps
I.Gro.
I.Cor.
Calibration Toolbox
Mo
Mo KA1/Tutorial
Std Dev: 0.013 %
0.021
Stat. error dominates standard deviation.
Redo
Undo
Off
On
Quadratic
Off
On
Tutorial.devm
Grap. Dis.
Standards
Line Over.
Summary
For Help, press F1
Status



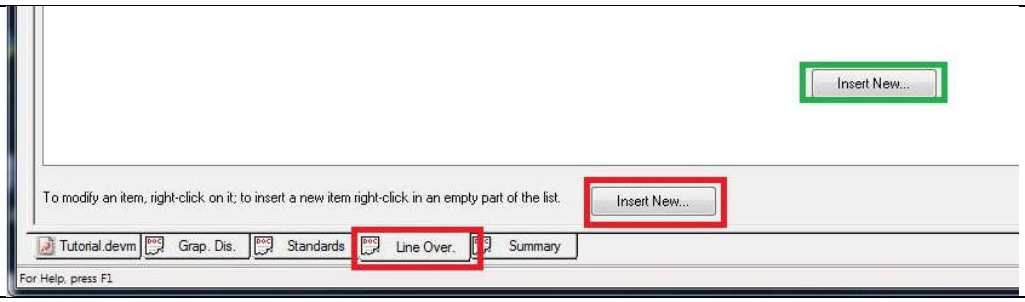
Select the columns to be displayed in the <Standards> panel



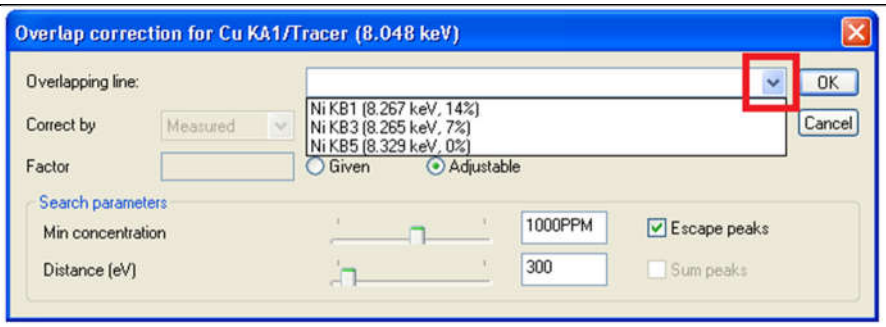
Select the next element (Cu) and click on the <Standards> tab. Note the “Std Dev.”



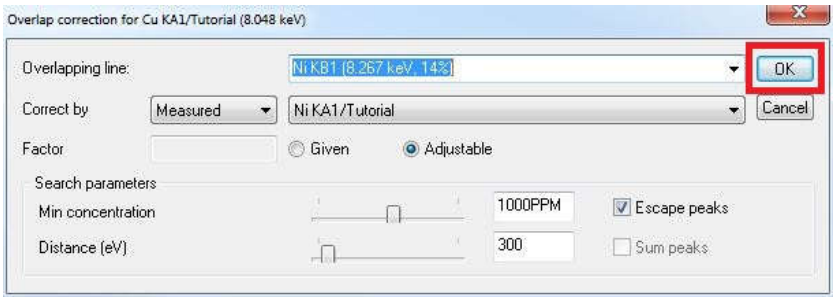
Sort the <Absolute Deviation> column and note that SS409 is the largest.

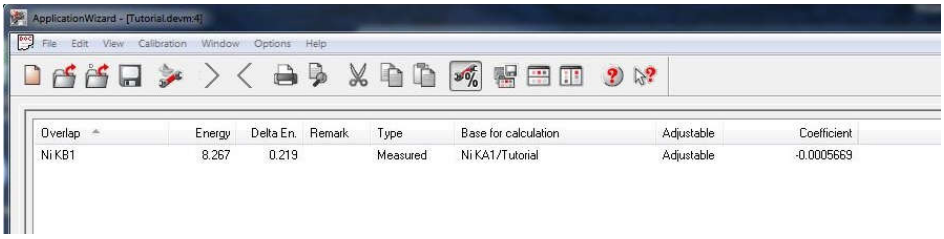


Select the <Line Over.> tab. Click on <Insert New…> or right-click on blank space to insert new.

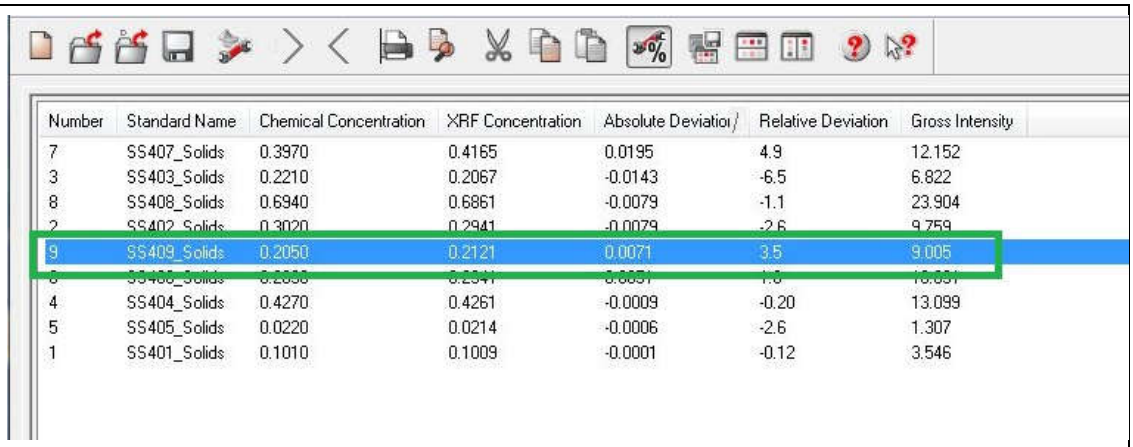


Select the best overlap suggestion (Ni KB1 in this case).



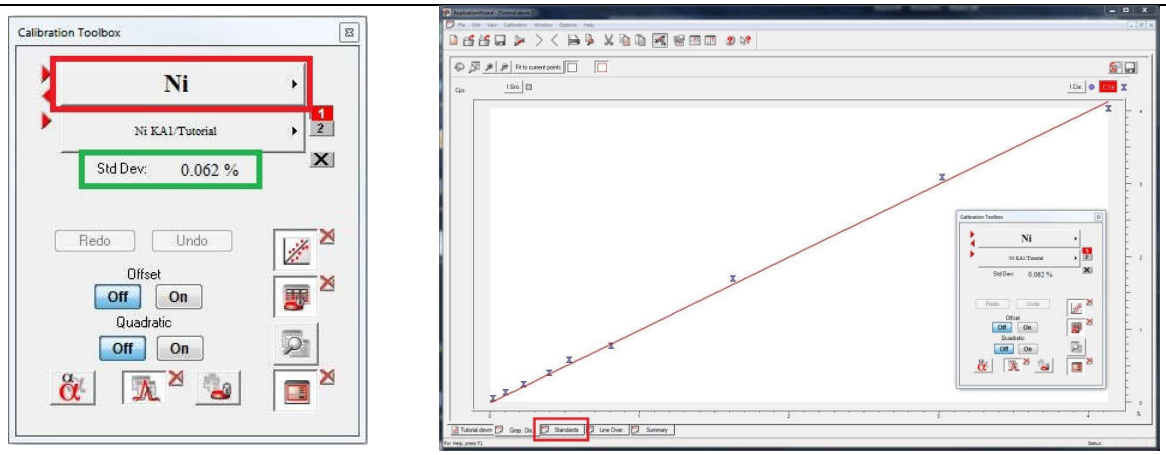


Note the line overlap is added to the table. To delete right click on the entry. Select the <Standards> tab.

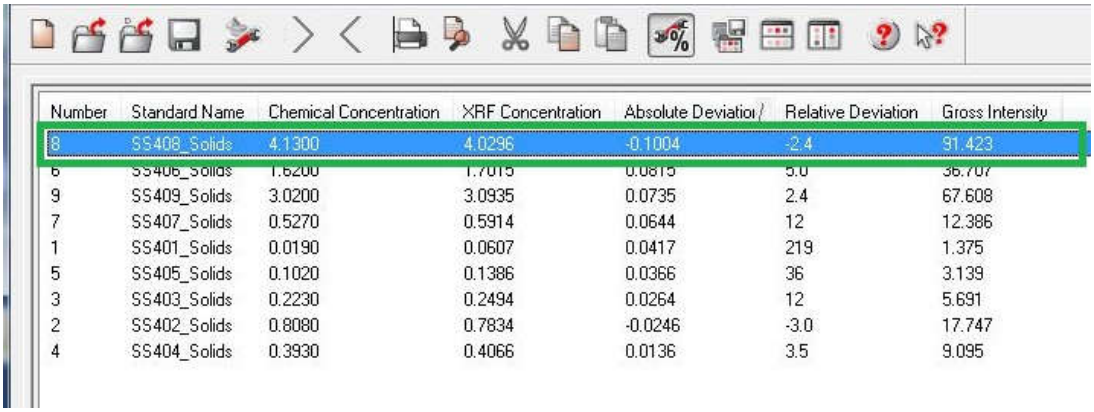


Number	Standard Name	Chemical Concentration	XRF Concentration	Absolute Deviation	Relative Deviation	Gross Intensity
7	SS407_Solids	0.3970	0.4165	0.0195	4.9	12.152
3	SS403_Solids	0.2210	0.2067	-0.0143	-6.5	6.822
8	SS408_Solids	0.6940	0.6861	-0.0079	-1.1	23.904
2	SS402_Solids	0.3020	0.2941	-0.0079	-2.6	9.759
9	SS409_Solids	0.2050	0.2121	0.0071	3.5	9.005
6	SS406_Solids	1.6200	1.6341	0.0141	1.0	36.697
4	SS404_Solids	0.4270	0.4261	-0.0009	-0.20	13.099
5	SS405_Solids	0.0220	0.0214	-0.0006	-2.6	1.307
1	SS401_Solids	0.1010	0.1009	-0.0001	-0.12	3.546

Note the <Absolute Deviation> is now 0.0071. Less than 1/3 of the “Std Dev.”

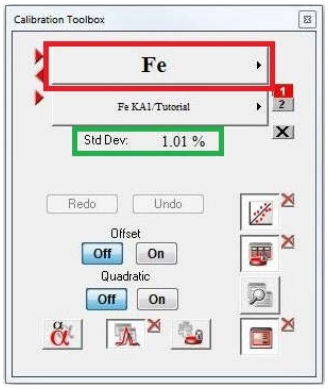


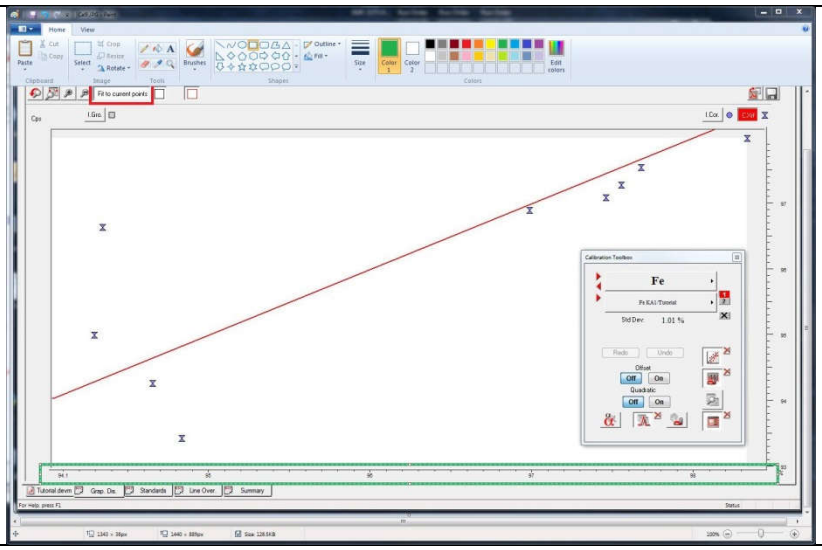
Next element (Ni). Note the “StdDev.” and select the <Standards> tab.



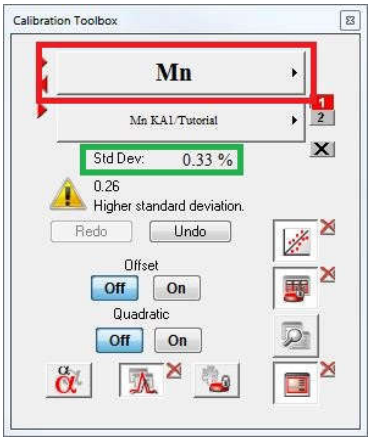
Number	Standard Name	Chemical Concentration	XRF Concentration	Absolute Deviation	Relative Deviation	Gross Intensity
8	SS408_Solids	4.1300	4.0296	-0.1004	-2.4	91.423
6	SS406_Solids	1.6200	1.7015	0.0815	5.0	36.707
9	SS409_Solids	3.0200	3.0935	0.0735	2.4	67.608
7	SS407_Solids	0.5270	0.5914	0.0644	12	12.386
1	SS401_Solids	0.0190	0.0607	0.0417	219	1.375
5	SS405_Solids	0.1020	0.1386	0.0366	36	3.139
3	SS403_Solids	0.2230	0.2494	0.0264	12	5.691
2	SS402_Solids	0.8080	0.7834	-0.0246	-3.0	17.747
4	SS404_Solids	0.3930	0.4066	0.0136	3.5	9.095

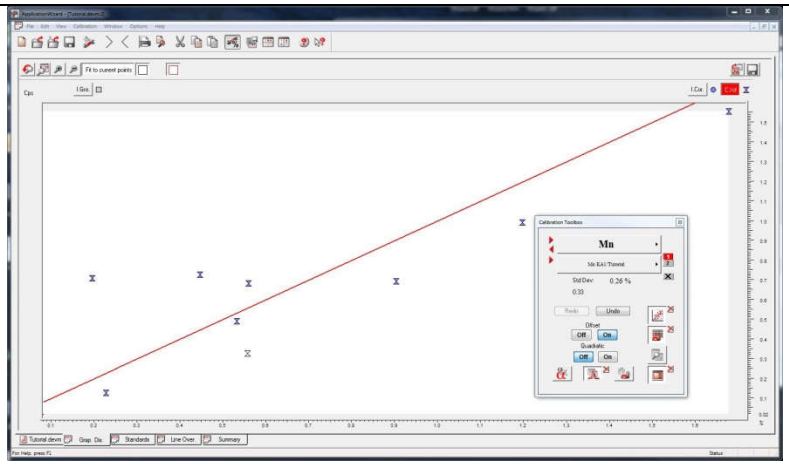
Note the <Absolute Deviation> is slightly larger than the “Std Dev.” However, when we go to the <Line Over.> tab there are no overlap suggestions.



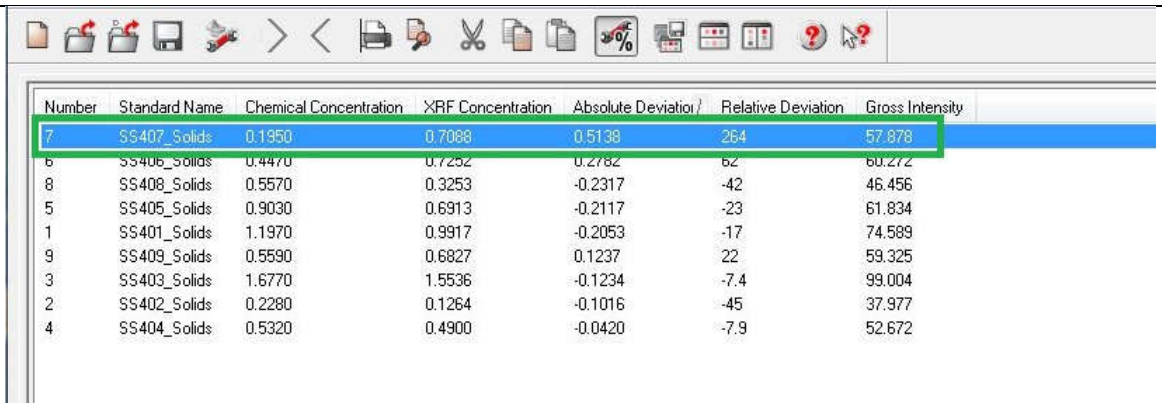


The next element is Fe. Note that in the figure we clicked <Fix to current point s>to adjust the x-axis. Fe is regarded as the matrix. Because Fe is calculated as the balance, while ignoring minor elements such as P, Si, N, it is inaccurate. We do not calibrate Fe.



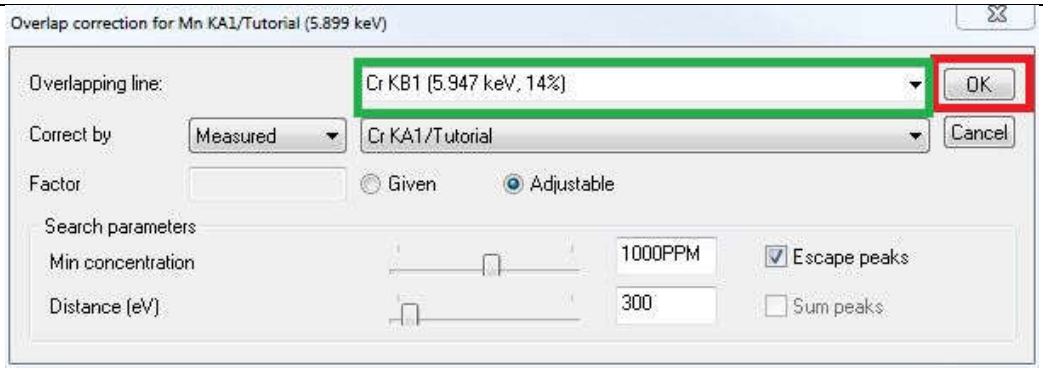


The next element is Mn. The “Std Dev.” is 0.33 %. The points are scattered.

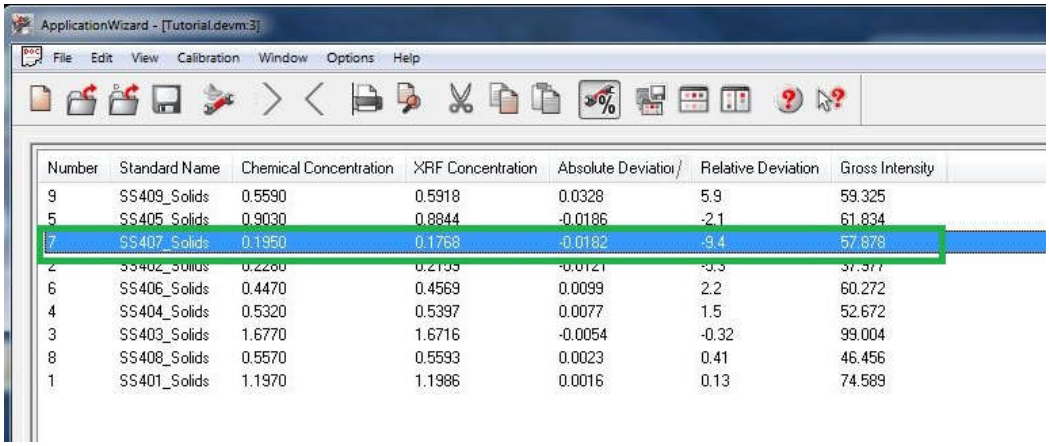


Number	Standard Name	Chemical Concentration	XRF Concentration	Absolute Deviation	Relative Deviation	Gross Intensity
7	SS407_Solids	0.1950	0.7088	0.5138	264	57.878
6	SS406_Solids	0.4470	0.7252	0.2782	62	60.272
8	SS408_Solids	0.5570	0.3253	-0.2317	-42	46.456
5	SS405_Solids	0.9030	0.6913	-0.2117	-23	61.834
1	SS401_Solids	1.1970	0.9917	-0.2053	-17	74.589
9	SS409_Solids	0.5590	0.6827	0.1237	22	59.325
3	SS403_Solids	1.6770	1.5536	-0.1234	-7.4	99.004
2	SS402_Solids	0.2280	0.1264	-0.1016	-45	37.977
4	SS404_Solids	0.5320	0.4900	-0.0420	-7.9	52.672

The<Absolute Deviation> is 0.5138 for SS407.

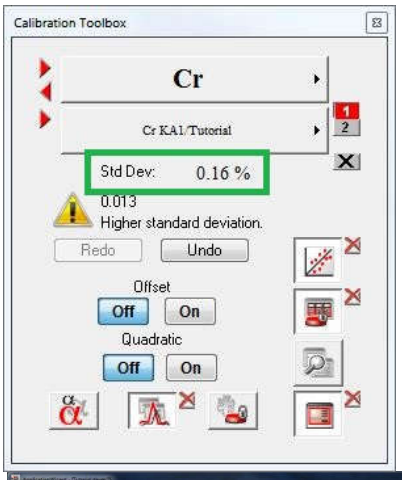


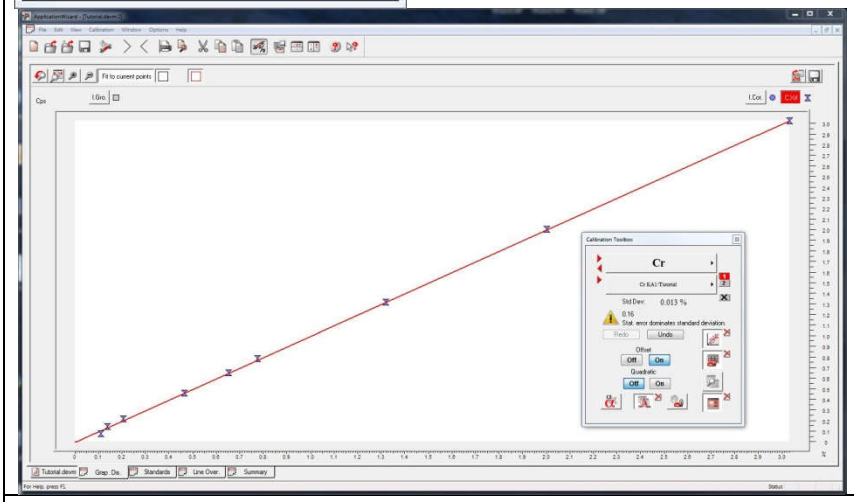
In the <Line Over.> tab insert the overlap as shown. It is inserted in the table.



Number	Standard Name	Chemical Concentration	XRF Concentration	Absolute Deviation	Relative Deviation	Gross Intensity
9	SS409_Solids	0.5590	0.5918	0.0328	5.9	59.325
5	SS405_Solids	0.9030	0.8844	-0.0186	-2.1	61.834
7	SS407_Solids	0.1950	0.1768	-0.0182	-9.4	57.878
2	SS402_Solids	0.2280	0.2155	-0.0121	-5.3	37.977
6	SS406_Solids	0.4470	0.4569	0.0099	2.2	60.272
4	SS404_Solids	0.5320	0.5397	0.0077	1.5	52.672
3	SS403_Solids	1.6770	1.6716	-0.0054	-0.32	99.004
8	SS408_Solids	0.5570	0.5593	0.0023	0.41	46.456
1	SS401_Solids	1.1970	1.1986	0.0016	0.13	74.589

The <Absolute Deviation> for SS407 is now down to 0.0182% and the largest one is still only 0.0328 %. Quite an improvement.

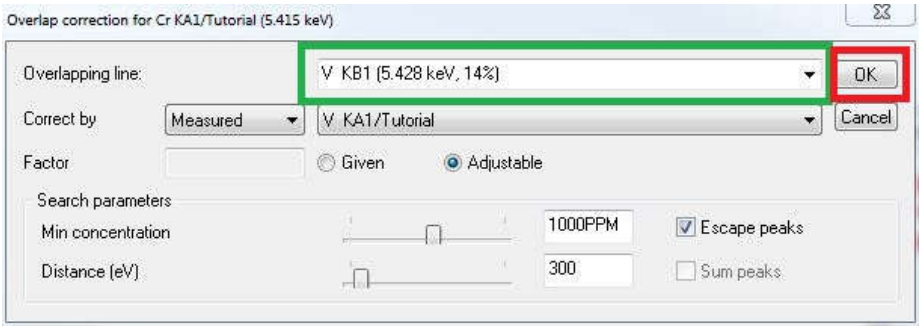




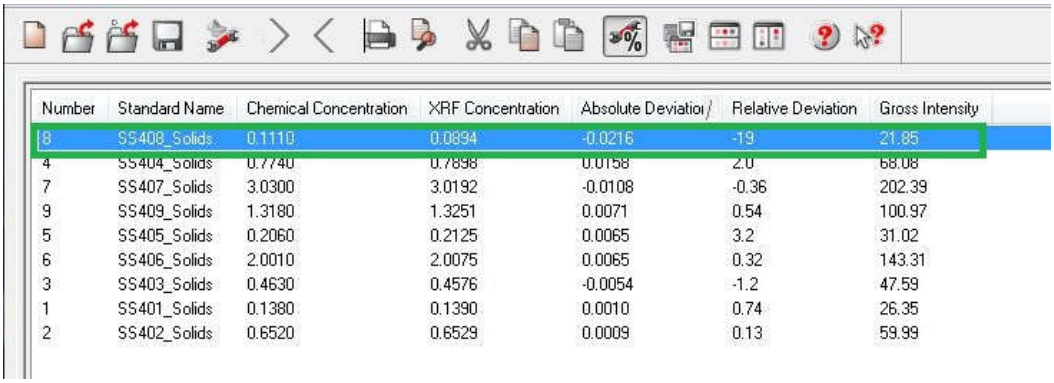
Next is Cr. Adding an offset improves the “Std Dev.” But let’s look at overlaps.

Number	Standard Name	Chemical Concentration	XRF Concentration	Absolute Deviation	Relative Deviation	Gross Intensity
8	SS408_Solids	0.1110	0.0811	-0.0299	-27	21.85
5	SS405_Solids	0.2060	0.2187	0.0127	6.2	31.02
4	SS404_Solids	0.7740	0.7852	0.0112	1.5	68.08
1	SS401_Solids	0.1380	0.1486	0.0106	7.7	26.35
7	SS407_Solids	3.0300	3.0251	-0.0049	-0.16	202.39
6	SS406_Solids	2.0010	2.0032	0.0022	0.11	143.31
3	SS403_Solids	0.4630	0.4610	-0.0020	-0.43	47.59
2	SS402_Solids	0.6520	0.6513	-0.0007	-0.11	59.99
9	SS409_Solids	1.3180	1.3187	0.0007	0.051	100.97

The largest<Absolute Deviation” is 0.0299.

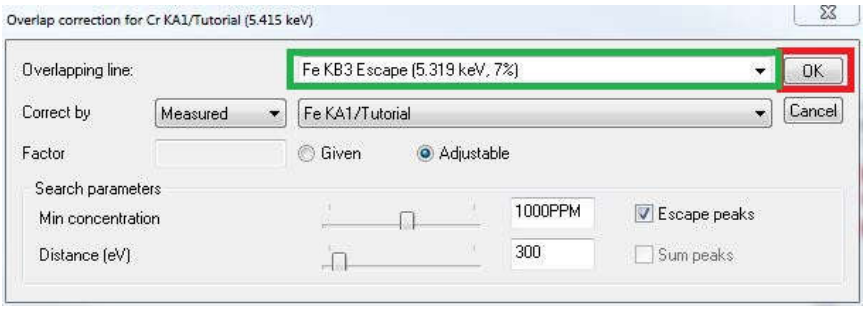


Select the V KB1 overlap, and click OK.

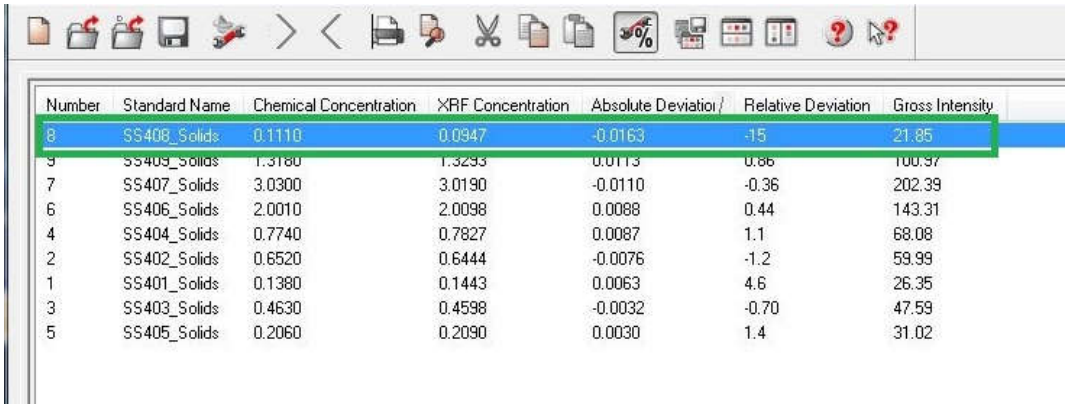


Number	Standard Name	Chemical Concentration	XRF Concentration	Absolute Deviation	Relative Deviation	Gross Intensity
8	SS408_Solids	0.1110	0.0894	-0.0216	-19	21.85
4	SS404_Solids	0.7740	0.7898	0.0158	2.0	68.08
7	SS407_Solids	3.0300	3.0192	-0.0108	-0.36	202.39
9	SS409_Solids	1.3180	1.3251	0.0071	0.54	100.97
5	SS405_Solids	0.2060	0.2125	0.0065	3.2	31.02
6	SS406_Solids	2.0010	2.0075	0.0065	0.32	143.31
3	SS403_Solids	0.4630	0.4576	-0.0054	-1.2	47.59
1	SS401_Solids	0.1380	0.1390	0.0010	0.74	26.35
2	SS402_Solids	0.6520	0.6529	0.0009	0.13	59.99

It only improve the <Absolute Deviation" from 0.0299 to 0.0200.

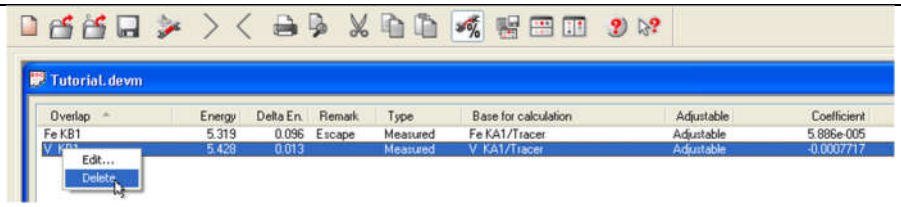


Next select the Fe Escape peak. And click OK.

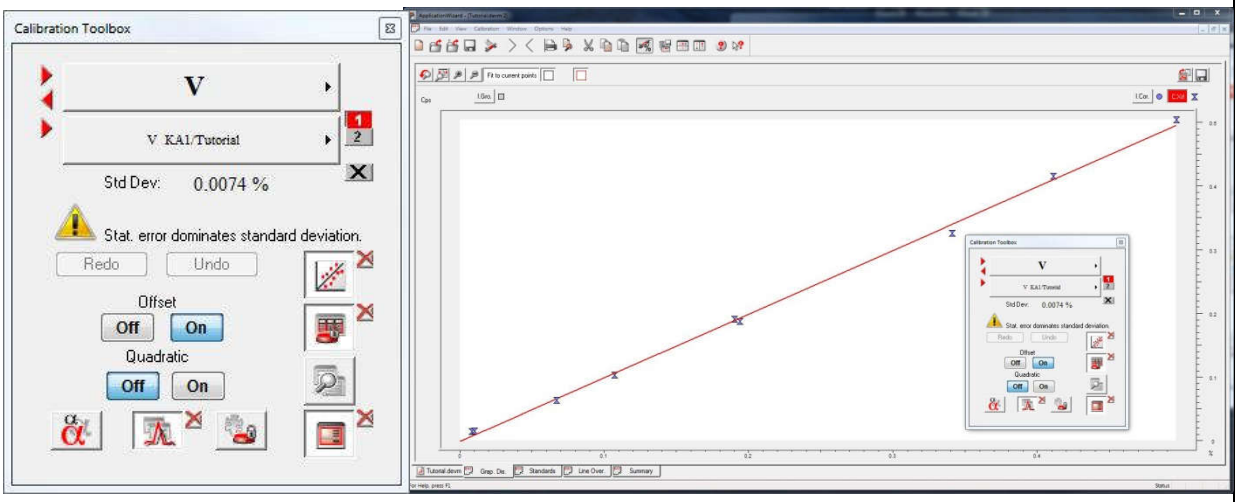


Number	Standard Name	Chemical Concentration	XRF Concentration	Absolute Deviation	Relative Deviation	Gross Intensity
8	SS408_Solids	0.1110	0.0947	-0.0163	-15	21.85
9	SS409_Solids	1.3180	1.3293	0.0113	0.86	100.97
7	SS407_Solids	3.0300	3.0190	-0.0110	-0.36	202.39
6	SS406_Solids	2.0010	2.0098	0.0088	0.44	143.31
4	SS404_Solids	0.7740	0.7827	0.0087	1.1	68.08
2	SS402_Solids	0.6520	0.6444	-0.0076	-1.2	59.99
1	SS401_Solids	0.1380	0.1443	0.0063	4.6	26.35
3	SS403_Solids	0.4630	0.4598	-0.0032	-0.70	47.59
5	SS405_Solids	0.2060	0.2090	0.0030	1.4	31.02

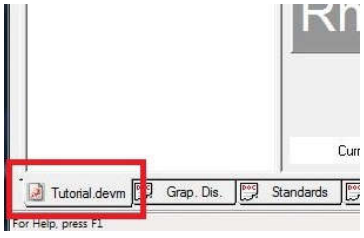
This again improves the deviations.

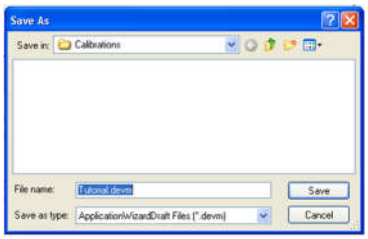


We therefore remove the V KB1. Because there is so much more Fe, its affect outweighs the V affect.



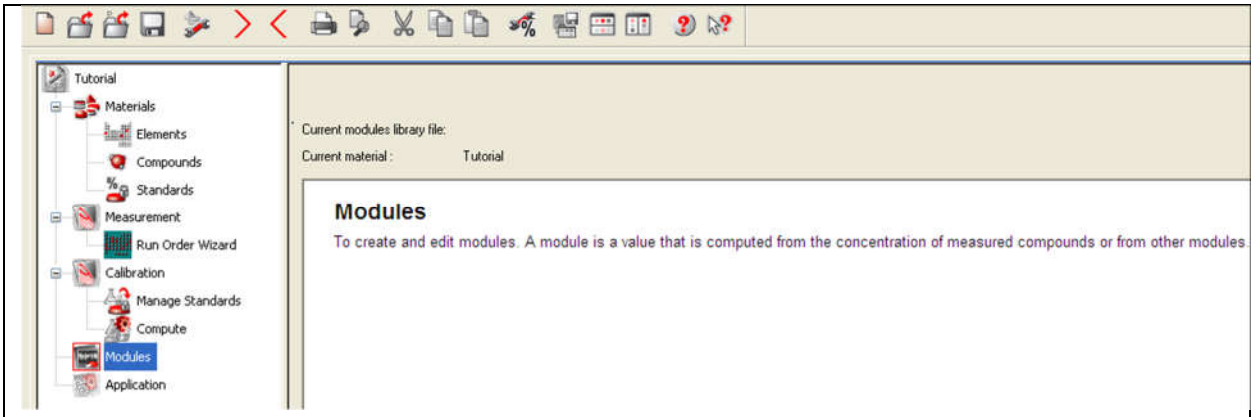
Next is V. It is already good.



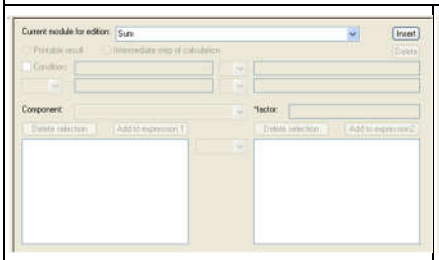


Select the left most tab, <Tutorial.devm>. Then click  . Click <Yes> to save the results.

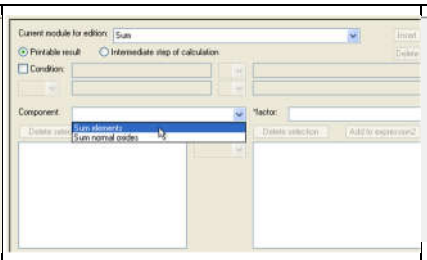
6. Modules.



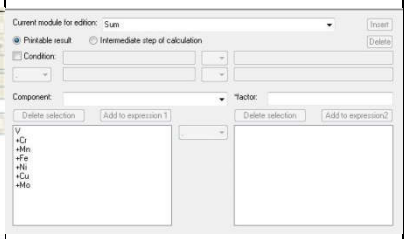
For Example:



Enter a name to show with results

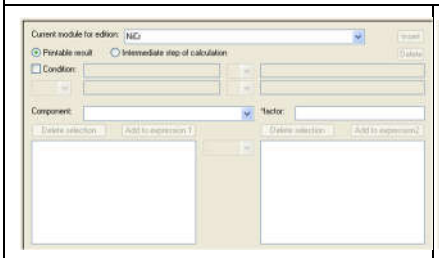


Select a function

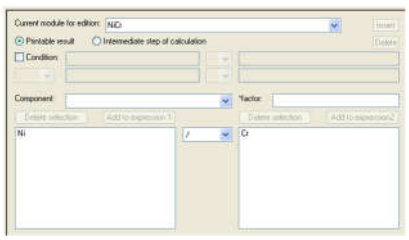


Enter the arguments

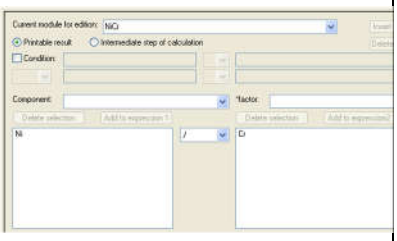
OR



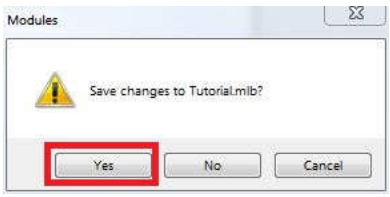
Enter a name to show with results

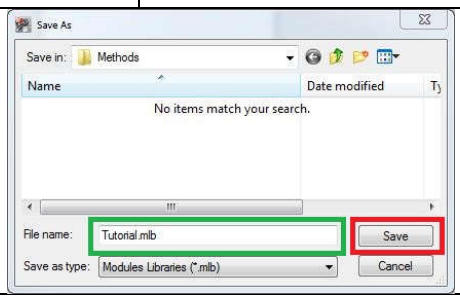


Select a condition



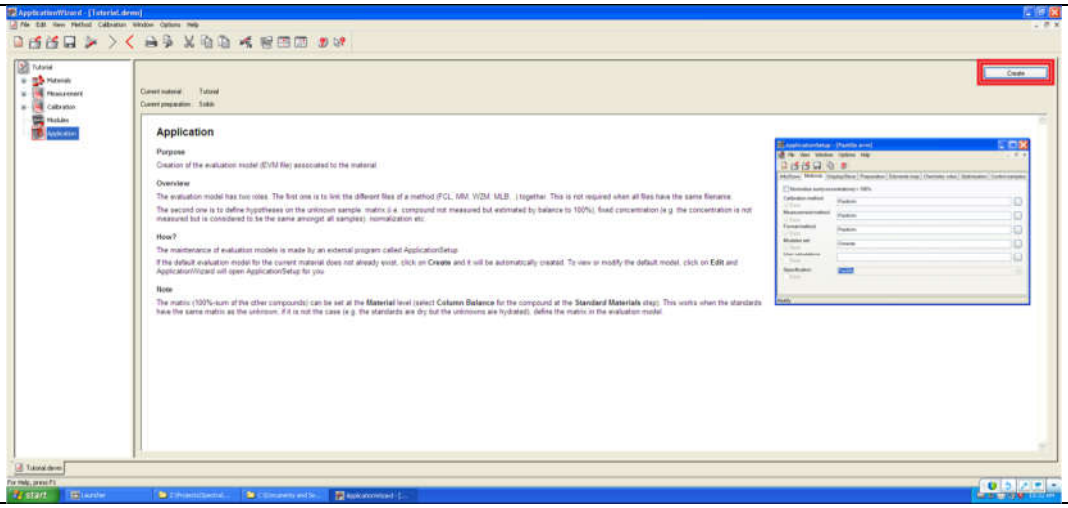
Enter the arguments

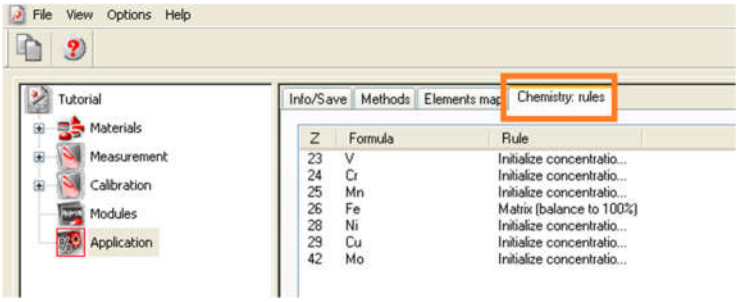




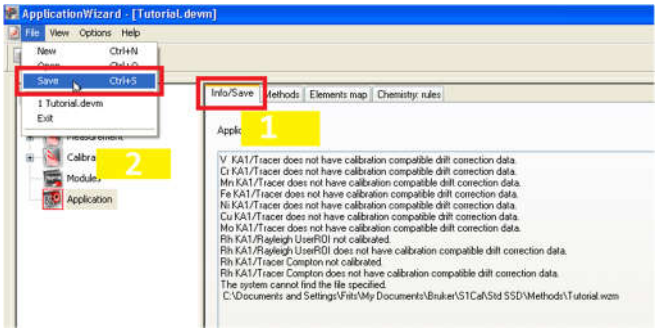
7. Saving the calibration.

7.1 The appinstall package.

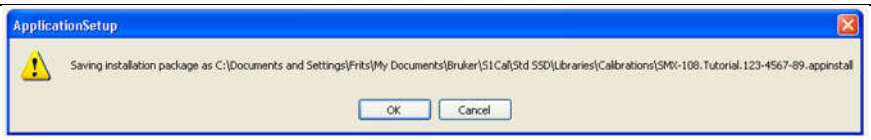




Check the <Chemistry Rules>

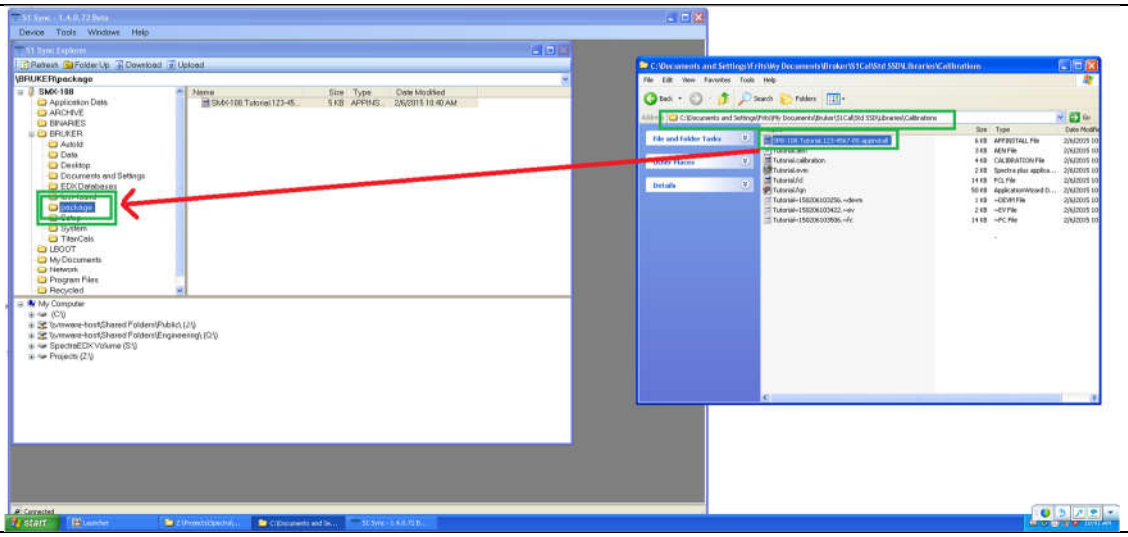


Select the <Info/Save> tab, then File -> Save to save the calibration installation package.

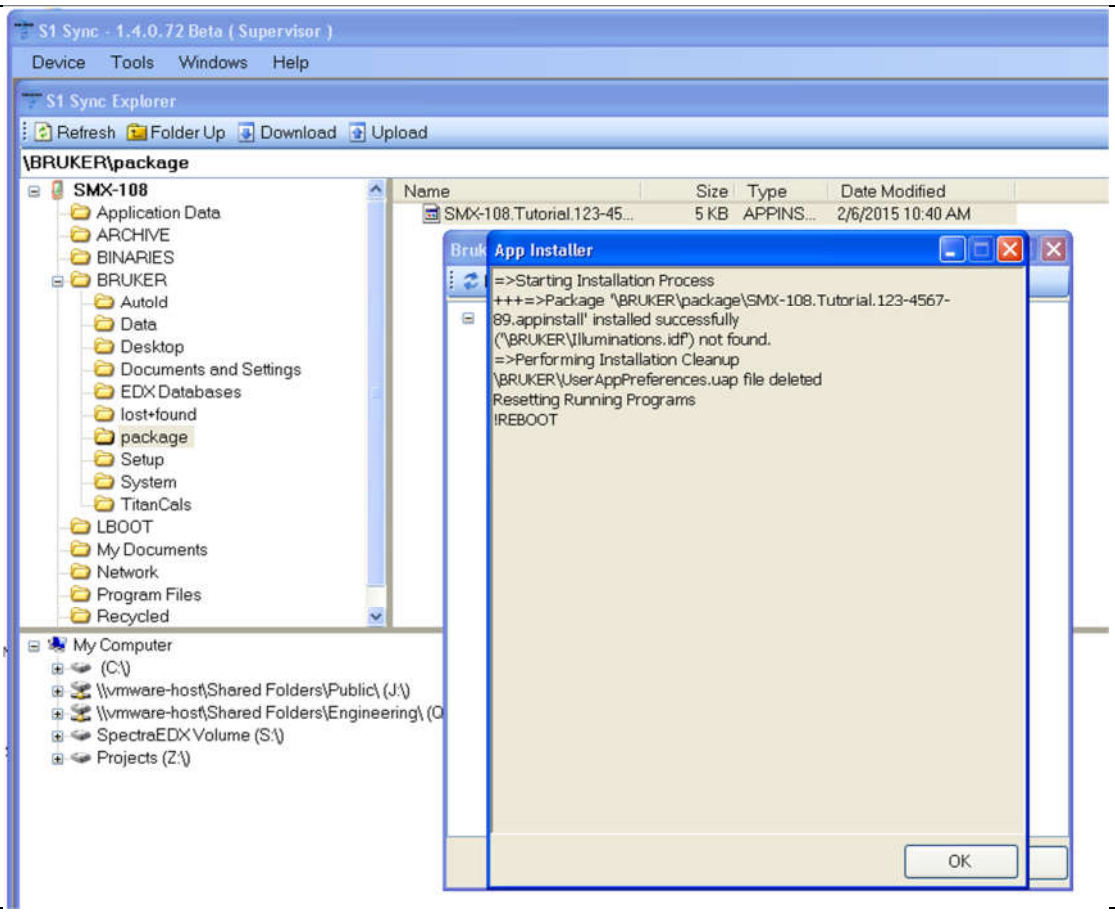


Note the folder as set by EasyCal where the appinstall package is stored.

7.2 Installing the appinstall package.

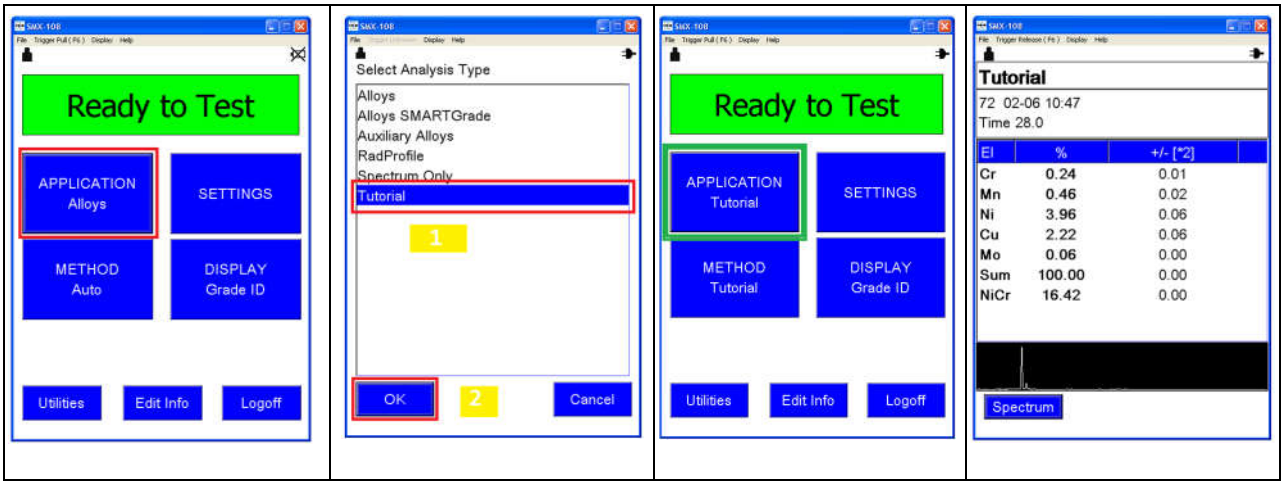


Open S1Sync, connect to the instrument. Open File Explorer and find the folder from 6.1.
Drag and drop the appinstall file on the package folder.



Select Tools -> Bruker Installer to install the appinstall package.

7.3 Testing the calibration.



Login to the instrument and click <APPLICATION>	Select the new calibration and click <OK>	Note that the new name is displayed in the <APPLICATION> button	Take an assay and note the concentrations as well as the Sum and Ni/Cr ratio are shown

The End