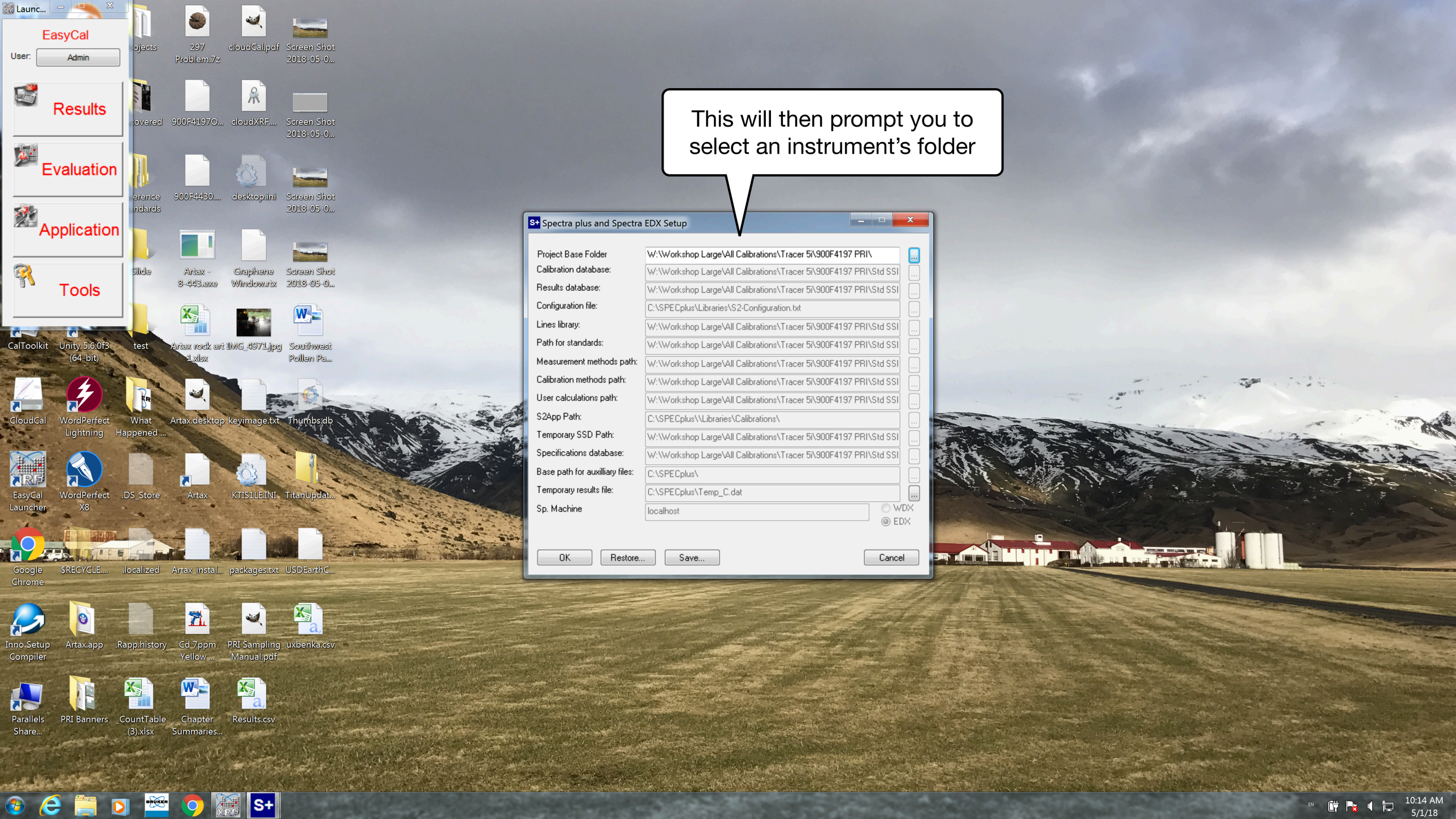
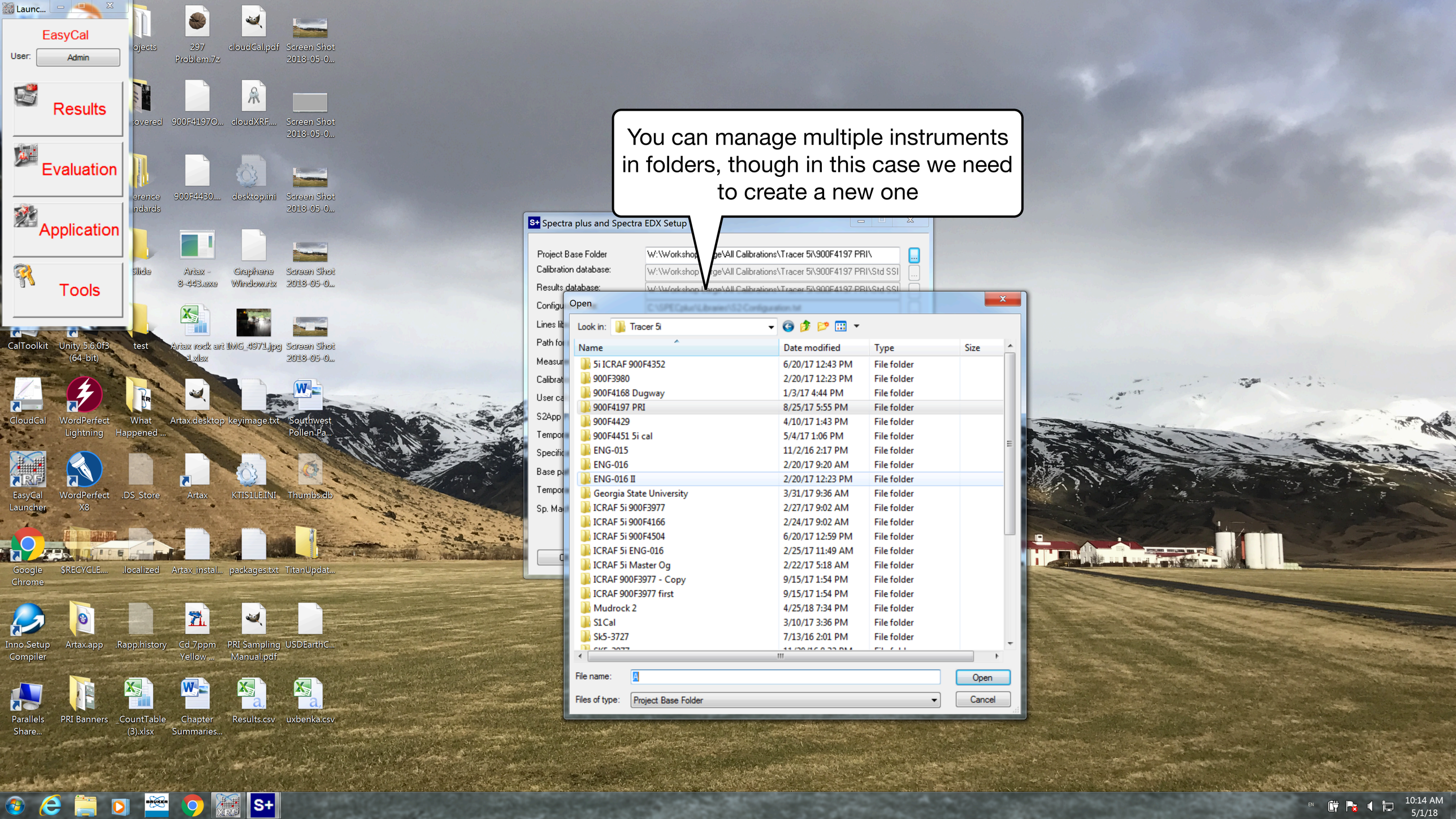
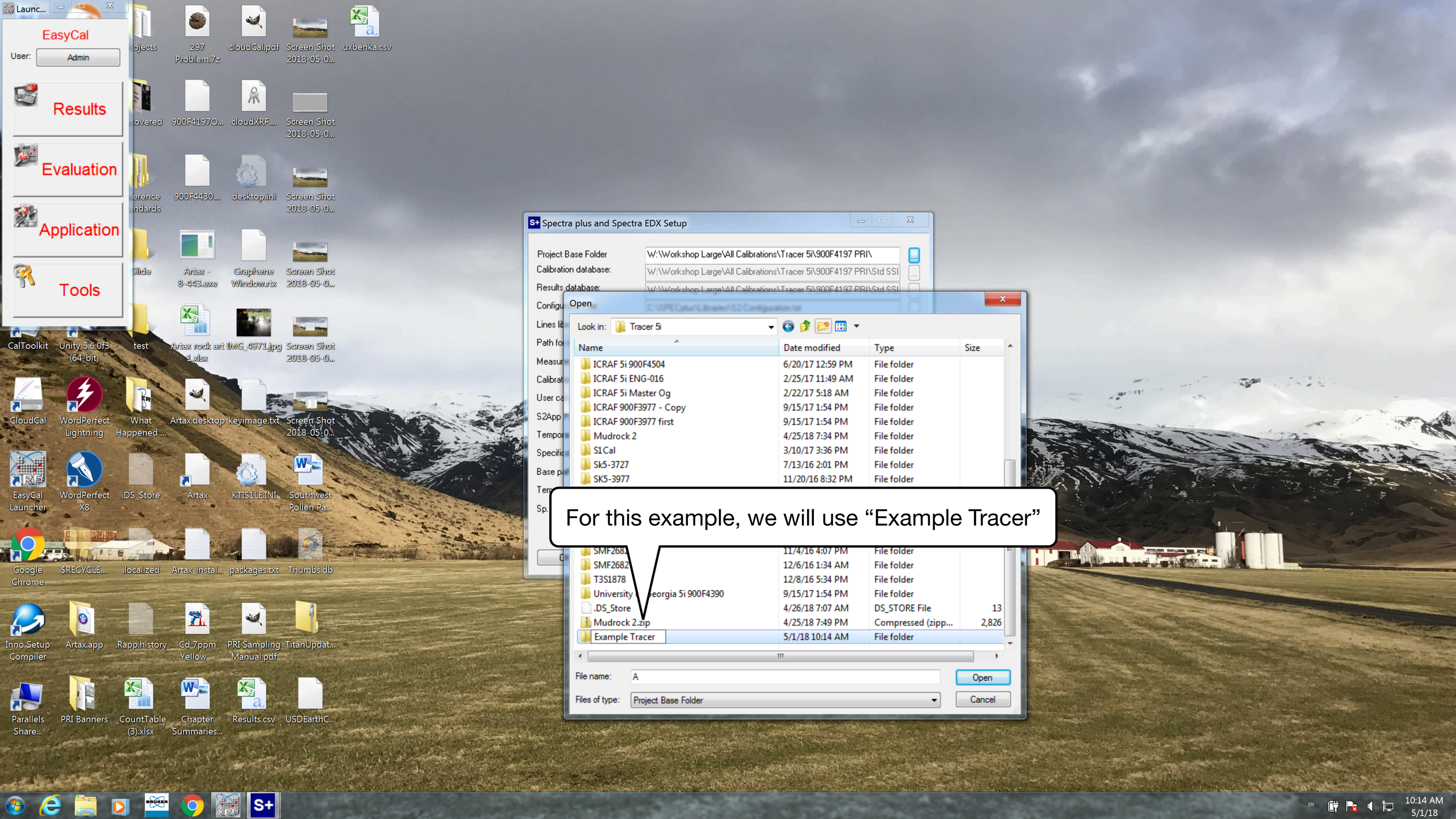
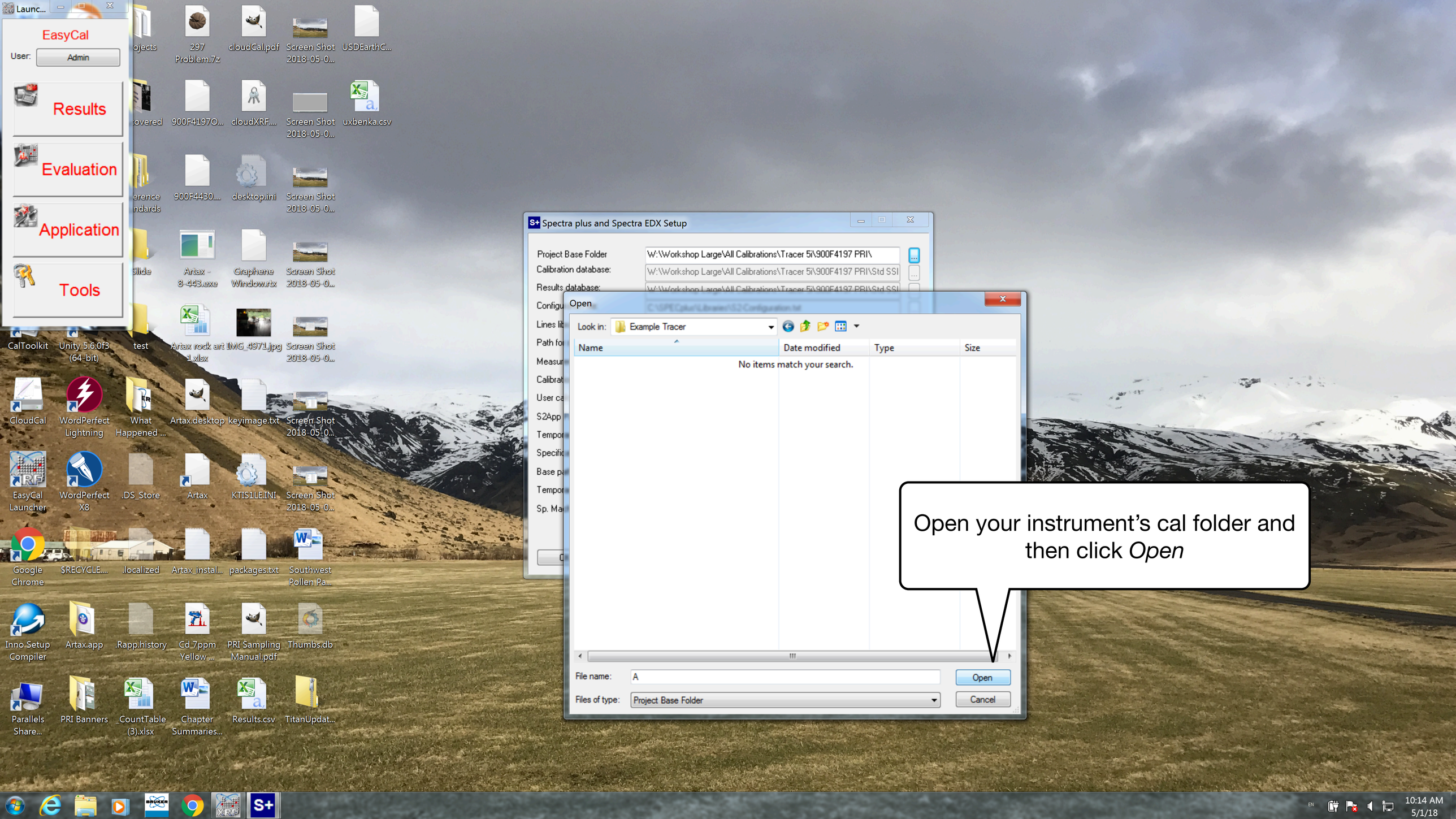

EasyCal
User:
Admin
Results
Evaluation
Application
Tools
Applications
Module Editor
PDZtoSSD
S1 Sync
S2Configuration
S2Setup
DumpSSD
Dump Method / Calibration
Go to *Tools* and then to *S2Setup*
To begin a new calibration for a new instrument, it is first necessary to set up that instrument. EasyCal functions by creating (and maintaining) folders for each instrument
To use EasyCal, we must maintain those folders

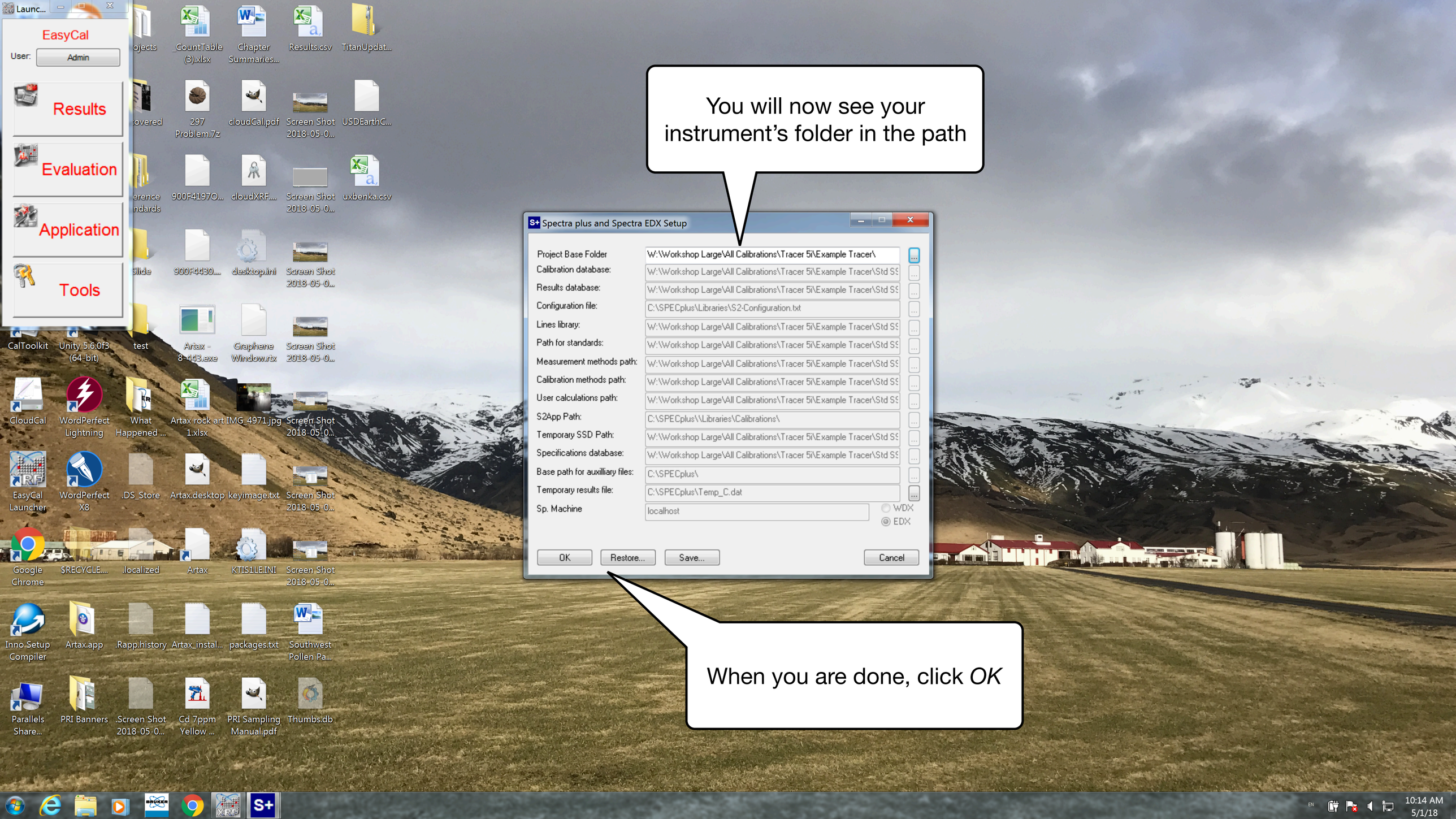

Launc...
EasyCal
User:
Admin
Results
Evaluation
Application
Tools
Make sure to select *EasyCal*
S+: Select Mode
EasyCal
Full SpectraEDX
OK
Cancel
297 Problem.7z
cloudCal.pdf
Screen Shot 2018-05-0...
900F4197O...
cloudXRF....
900F4430....
desktop.ini
Artax - 8-443.exe
Graphene Window.rtx
Southwest Pollen Pa...
Artax rock art 1.xlsx
IMG_4971.jpg
Thumbs.db
CalToolkit
Unity 5.6.0f3 (64-bit)
test
CloudCal
WordPerfect Lightning
What Happened ...
Artax.desktop
keyimage.txt
TitanUpdat...
EasyCal Launcher
WordPerfect X8
.DS_Store
Artax
KTIS1LE.INI
USDEarthC...
Google Chrome
$RECYCLE....
.localized
Artax_instal...
packages.txt
uxbenka.csv
Inno Setup Compiler
Artax.app
.Rapp.history
Cd 7ppm Yellow ...
PRI Sampling Manual.pdf
Parallels Share...
PRI Banners
_CountTable (3).xlsx
Chapter Summaries...
Results.csv
10:11 AM
5/1/18

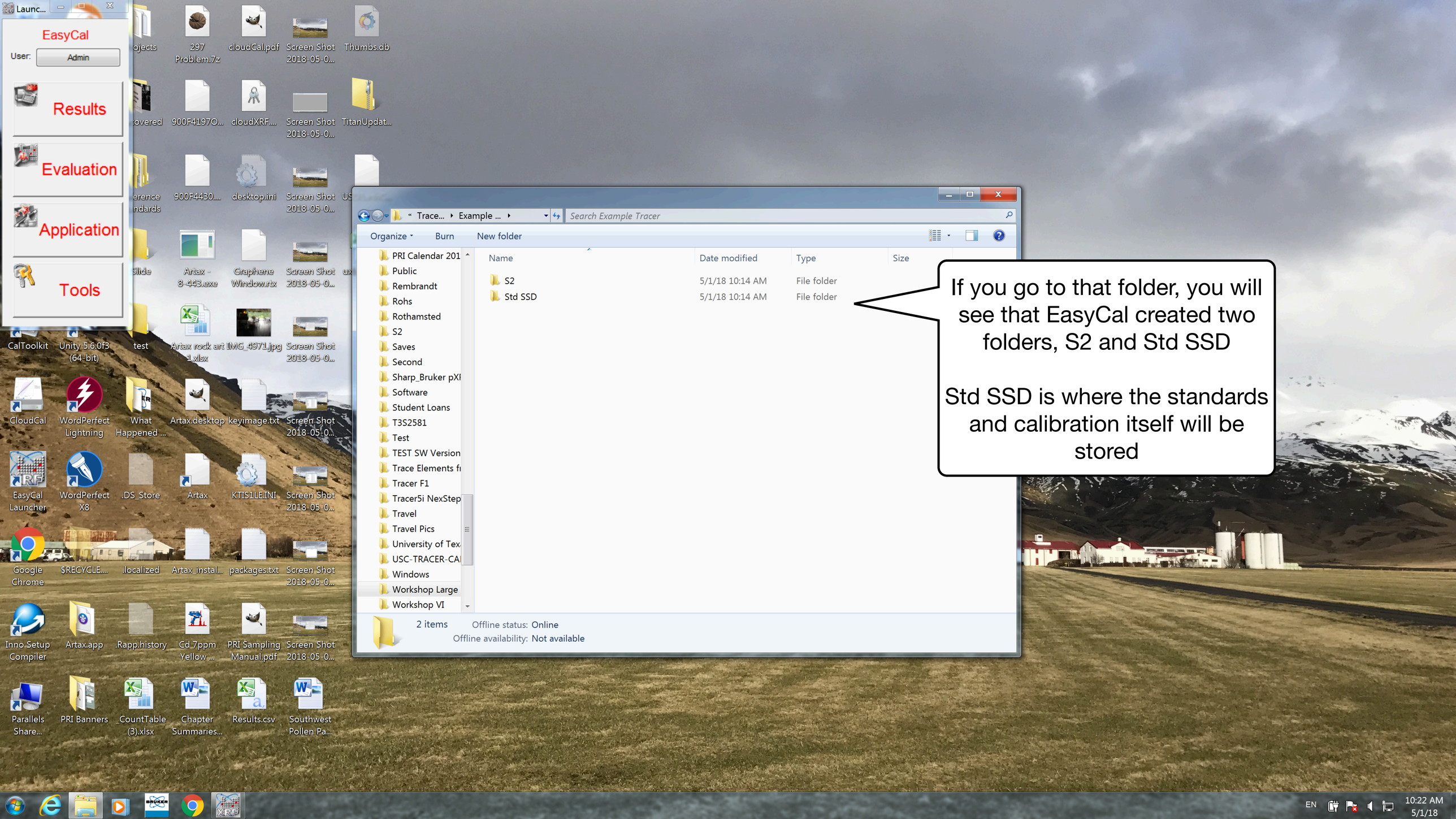

EasyCal
User:
Admin
Results
Evaluation
Application
Tools
This will then prompt you to select an instrument's folder
Spectra plus and Spectra EDX Setup
Project Base Folder
W:\Workshop Large\All Calibrations\Tracer 5i\900F4197 PRI\
Calibration database:
Results database:
Configuration file:
C:\SPECplus\Libraries\S2-Configuration.txt
Lines library:
Path for standards:
Measurement methods path:
Calibration methods path:
User calculations path:
S2App Path:
C:\SPECplus\\Libraries\Calibrations\
Temporary SSD Path:
Specifications database:
Base path for auxilliary files:
C:\SPECplus\
Temporary results file:
C:\SPECplus\Temp_C.dat
Sp. Machine
localhost
WDX
EDX
OK
Restore...
Save...
Cancel


EasyCal
User:
Admin
Results
Evaluation
Application
Tools
You can manage multiple instruments in folders, though in this case we need to create a new one
Spectra plus and Spectra EDX Setup
Project Base Folder
Calibration database:
Results database:
Open
Look in:
Tracer 5i
Name
Date modified
Type
Size
5i ICRAF 900F4352 6/20/17 12:43 PM File folder
900F3980 2/20/17 12:23 PM File folder
900F4168 Dugway 1/3/17 4:44 PM File folder
900F4197 PRI 8/25/17 5:55 PM File folder
900F4429 4/10/17 1:43 PM File folder
900F4451 5i cal 5/4/17 1:06 PM File folder
ENG-015 11/2/16 2:17 PM File folder
ENG-016 2/20/17 9:20 AM File folder
ENG-016 II 2/20/17 12:23 PM File folder
Georgia State University 3/31/17 9:36 AM File folder
ICRAF 5i 900F3977 2/27/17 9:02 AM File folder
ICRAF 5i 900F4166 2/24/17 9:02 AM File folder
ICRAF 5i 900F4504 6/20/17 12:59 PM File folder
ICRAF 5i ENG-016 2/25/17 11:49 AM File folder
ICRAF 5i Master Og 2/22/17 5:18 AM File folder
ICRAF 900F3977 - Copy 9/15/17 1:54 PM File folder
ICRAF 900F3977 first 9/15/17 1:54 PM File folder
Mudrock 2 4/25/18 7:34 PM File folder
S1Cal 3/10/17 3:36 PM File folder
Sk5-3727 7/13/16 2:01 PM File folder
File name:
Open
Files of type:
Project Base Folder
Cancel
CalToolkit
Unity 5.6.0f3 (64-bit)
test
Artax rock art 1.xlsx
IMG_4971.jpg
Screen Shot 2018-05-0...
CloudCal
WordPerfect Lightning
What Happened ...
Artax.desktop
keyimage.txt
Southwest Pollen Pa...
EasyCal Launcher
WordPerfect X8
.DS_Store
Artax
KTIS1LE.INI
Thumbs.db
Google Chrome
$RECYCLE....
.localized
Artax_instal...
packages.txt
TitanUpdat...
Inno Setup Compiler
Artax.app
.Rapp.history
Cd 7ppm Yellow ...
PRI Sampling Manual.pdf
USDEarthC...
Parallels Share...
PRI Banners
_CountTable (3).xlsx
Chapter Summaries...
Results.csv
uxbenka.csv
10:14 AM
5/1/18


EasyCal
User:
Admin
Results
Evaluation
Application
Tools
Spectra plus and Spectra EDX Setup
Project Base Folder
W:\Workshop Large\All Calibrations\Tracer 5i\900F4197 PRI\
Calibration database:
W:\Workshop Large\All Calibrations\Tracer 5i\900F4197 PRI\Std SSI
Results database:
Open
Look in:
Tracer 5i
Name
Date modified
Type
Size
ICRAF 5i 900F4504 6/20/17 12:59 PM File folder
ICRAF 5i ENG-016 2/25/17 11:49 AM File folder
ICRAF 5i Master Og 2/22/17 5:18 AM File folder
ICRAF 900F3977 - Copy 9/15/17 1:54 PM File folder
ICRAF 900F3977 first 9/15/17 1:54 PM File folder
Mudrock 2 4/25/18 7:34 PM File folder
S1Cal 3/10/17 3:36 PM File folder
Sk5-3727 7/13/16 2:01 PM File folder
SK5-3977 11/20/16 8:32 PM File folder
SMF2682 12/6/16 1:34 AM File folder
T3S1878 12/8/16 5:34 PM File folder
.DS_Store 4/26/18 7:07 AM DS_STORE File 13
Mudrock 2.zip 4/25/18 7:49 PM Compressed (zipp... 2,826
Example Tracer 5/1/18 10:14 AM File folder
File name:
A
Open
Files of type:
Project Base Folder
Cancel
For this example, we will use “Example Tracer”


Launc...
EasyCal
User:
Admin
Results
Evaluation
Application
Tools
Spectra plus and Spectra EDX Setup
Project Base Folder
W:\Workshop Large\All Calibrations\Tracer 5i\900F4197 PRI\
Calibration database:
W:\Workshop Large\All Calibrations\Tracer 5i\900F4197 PRI\Std SSI
Results database:
Open
Look in:
Example Tracer
Name
Date modified
Type
Size
No items match your search.
File name:
A
Open
Files of type:
Project Base Folder
Cancel
Open your instrument's cal folder and then click *Open*
CalToolkit
Unity 5.6.0f3 (64-bit)
test
Artax rock art 1.xlsx
IMG_4971.jpg
Screen Shot 2018-05-0...
CloudCal
WordPerfect Lightning
What Happened ...
Artax.desktop
keyimage.txt
EasyCal Launcher
WordPerfect X8
.DS_Store
Artax
KTIS1LE.INI
Google Chrome
$RECYCLE....
.localized
Artax_instal...
packages.txt
Southwest Pollen Pa...
Inno Setup Compiler
Artax.app
.Rapp.history
Cd 7ppm Yellow ...
PRI Sampling Manual.pdf
Thumbs.db
Parallels Share...
PRI Banners
_CountTable (3).xlsx
Chapter Summaries...
Results.csv
TitanUpdat...
297 Problem.7z
cloudCal.pdf
USDEarthC...
900F4197O...
cloudXRF....
uxbenka.csv
900F4430....
desktop.ini
Artax - 8-443.exe
Graphene Window.rtx
10:14 AM
5/1/18

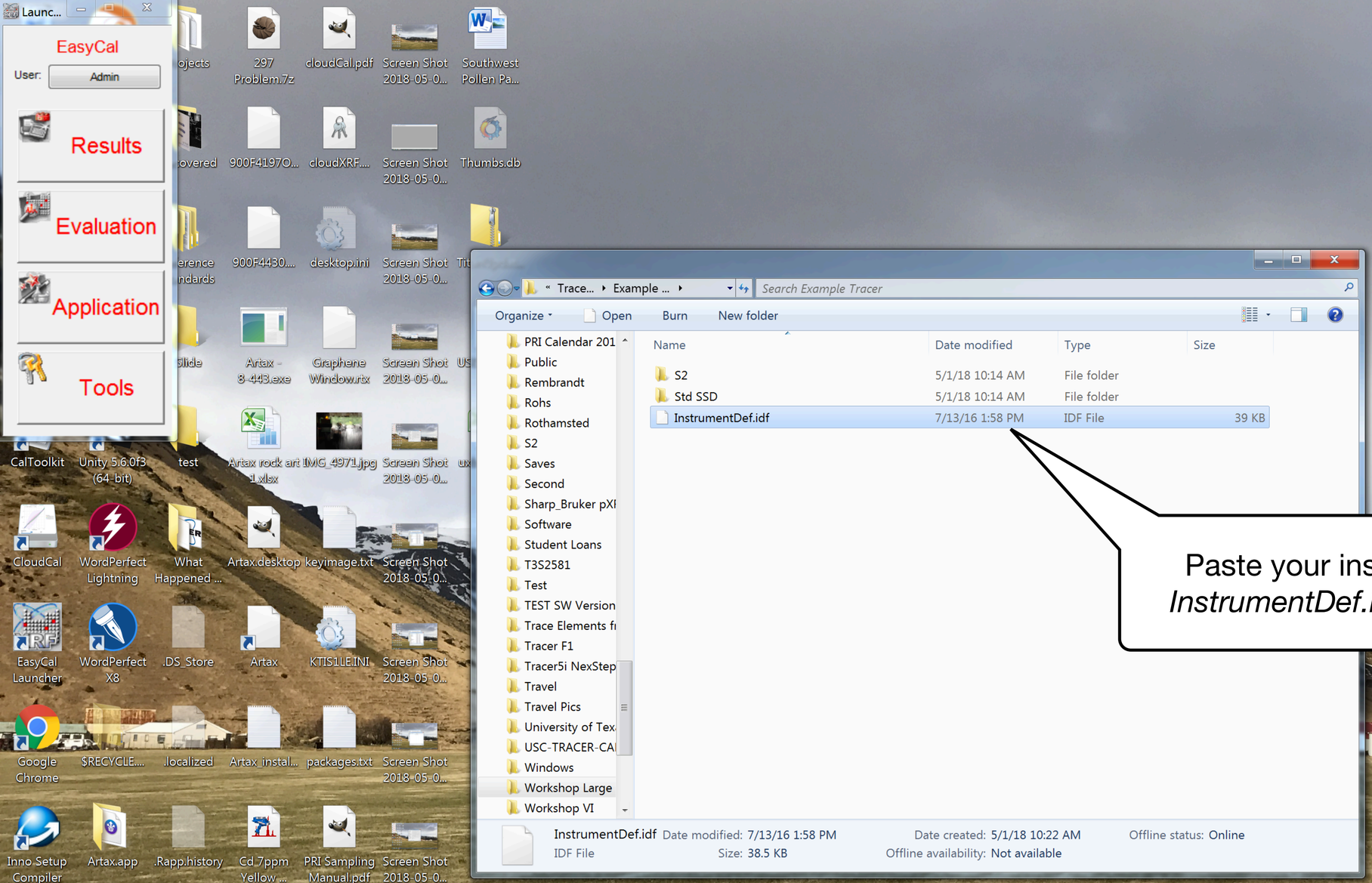

EasyCal
User:
Admin
Results
Evaluation
Application
Tools
Spectra plus and Spectra EDX Setup
Project Base Folder
W:\Workshop Large\All Calibrations\Tracer 5i\Example Tracer\
Calibration database:
Results database:
Configuration file:
C:\SPECplus\Libraries\S2-Configuration.txt
Lines library:
Path for standards:
Measurement methods path:
Calibration methods path:
User calculations path:
S2App Path:
C:\SPECplus\\Libraries\Calibrations\
Temporary SSD Path:
Specifications database:
Base path for auxilliary files:
C:\SPECplus\
Temporary results file:
C:\SPECplus\Temp_C.dat
Sp. Machine
localhost
WDX
EDX
OK
Restore...
Save...
Cancel
You will now see your instrument's folder in the path
When you are done, click OK

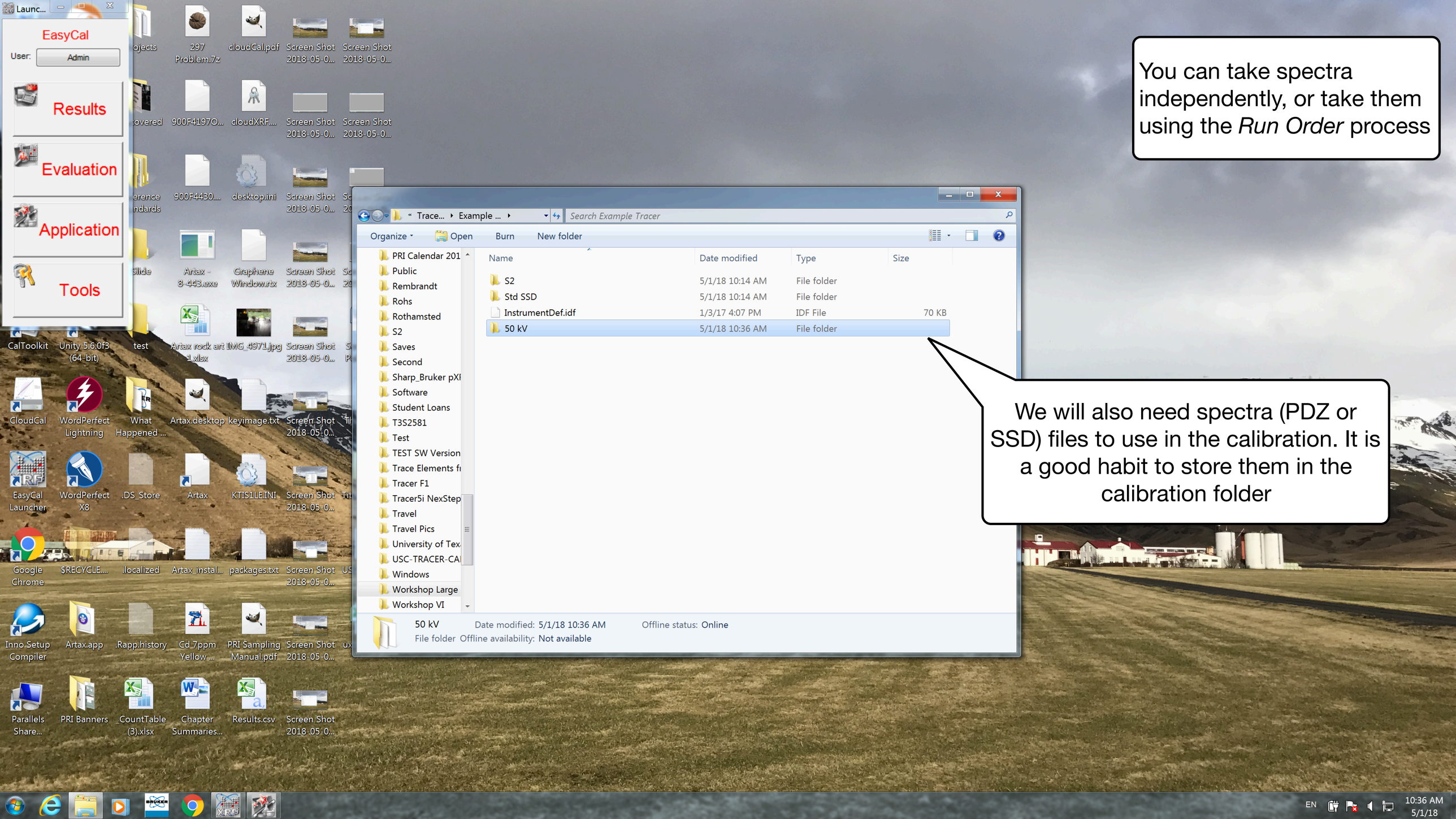

EasyCal
User:
Admin
Results
Evaluation
Application
Tools
Trace... ▸ Example ... ▸
Search Example Tracer
Organize
Burn
New folder
PRI Calendar 201
Public
Rembrandt
Rohs
Rothamsted
S2
Saves
Second
Sharp_Bruker pXI
Software
Student Loans
T3S2581
Test
TEST SW Version
Trace Elements fi
Tracer F1
Tracer5i NexStep
Travel
Travel Pics
University of Tex
USC-TRACER-CA
Windows
Workshop Large
Workshop VI
Name
Date modified
Type
Size
S2
5/1/18 10:14 AM
File folder
Std SSD
5/1/18 10:14 AM
File folder
2 items
Offline status: Online
Offline availability: Not available
If you go to that folder, you will see that EasyCal created two folders, S2 and Std SSD
Std SSD is where the standards and calibration itself will be stored

Each Tracer, Titan, XMS, and CTX has an *InstrumentDef.idf* file. It is crucial to make sure it is in the calibration folder

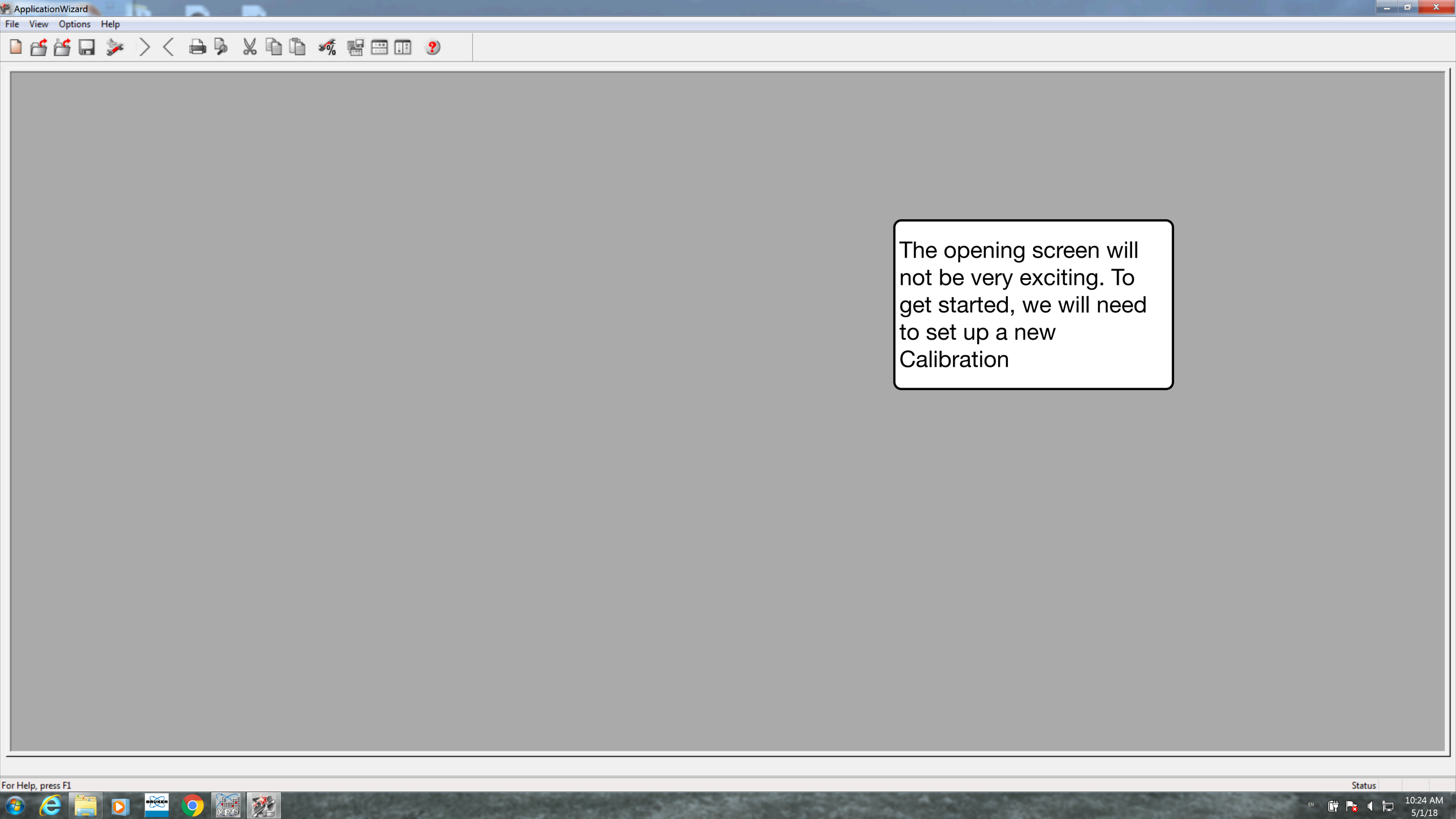
It is stored on your instrument itself under / Bruker/InstrumentDef.idf. Copy and paste it using *BIT* or a *USB*

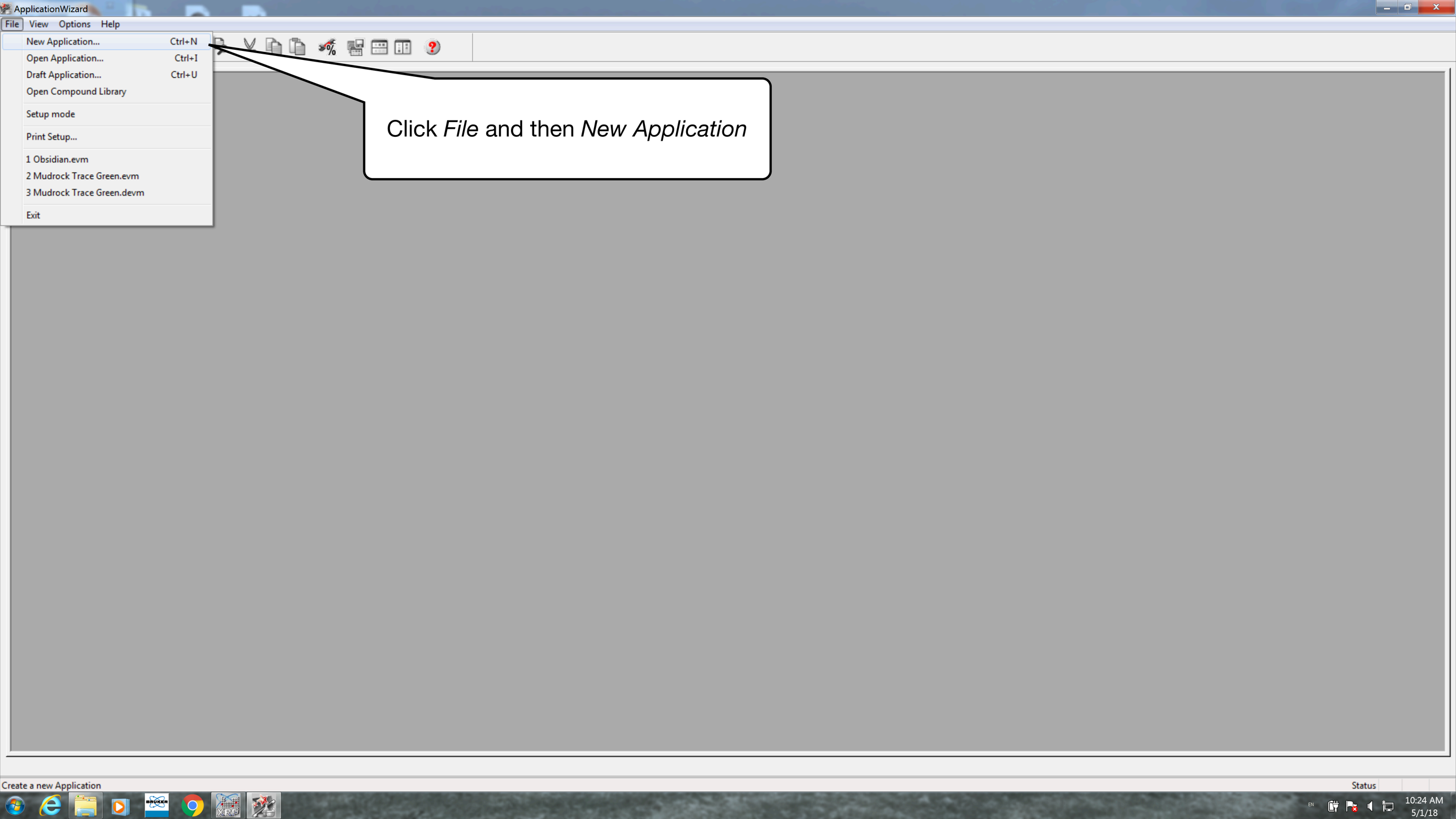
Paste your instrument's *InstrumentDef.idf* file here

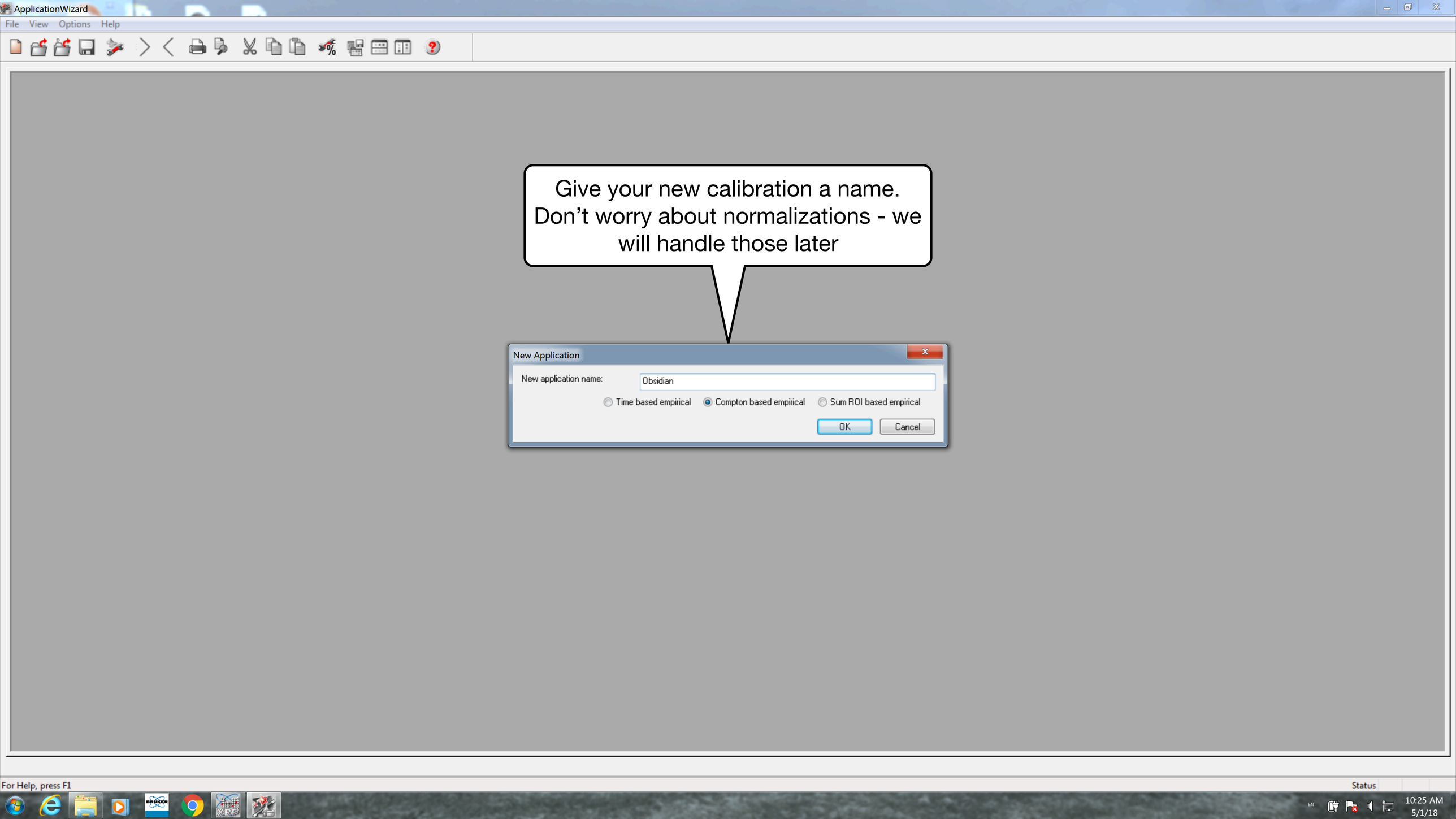



EasyCal
User:
Admin
Results
Evaluation
Application
Tools
Trace... ▸ Example ... ▸
Search Example Tracer
Organize
Open
Burn
New folder
Name
Date modified
Type
Size
S2
5/1/18 10:14 AM
File folder
Std SSD
5/1/18 10:14 AM
File folder
InstrumentDef.idf
1/3/17 4:07 PM
IDF File
70 KB
50 kV
5/1/18 10:36 AM
File folder
PRI Calendar 201
Public
Rembrandt
Rohs
Rothamsted
S2
Saves
Second
Sharp_Bruker pXF
Software
Student Loans
T3S2581
Test
TEST SW Version
Trace Elements f
Tracer F1
Tracer5i NexStep
Travel
Travel Pics
University of Tex
USC-TRACER-CA
Windows
Workshop Large
Workshop VI
50 kV
Date modified: 5/1/18 10:36 AM
Offline status: Online
File folder
Offline availability: Not available
You can take spectra independently, or take them using the Run Order process
We will also need spectra (PDZ or SSD) files to use in the calibration. It is a good habit to store them in the calibration folder


Launc...
EasyCal
User:
Admin
Results
Evaluation
Application
Calibration wizard
Tools
When you are ready to proceed, click *Application*
Banners
_CountTable (3).xlsx
Chapter Summaries...
Results.csv
ojects
297 Problem.7z
cloudCal.pdf
Southwest Pollen Pa...
overed
900F4197O...
cloudXRF....
Thumbs.db
ndards
CalToolkit
Unity 5.6.0f3 (64-bit)
Slide
Artax - 8-443.exe
Graphene Window.rtx
CloudCal
WordPerfect Lightning
test
Artax rock art 1.xlsx
IMG_4971.jpg
uxbenka.csv
EasyCal Launcher
WordPerfect X8
What Happened ...
Artax.desktop
keyimage.txt
Google Chrome
$RECYCLE....
.DS_Store
Artax
KTIS1LE.INI
Inno Setup Compiler
Artax.app
.localized
Artax_instal...
packages.txt
Parallels Share...
EasyCal Screenshots
.Rapp.history
Cd 7ppm Yellow ...
PRI Sampling Manual.pdf
11:41 AM
5/1/18


ApplicationWizard
File
View
Options
Help
The opening screen will not be very exciting. To get started, we will need to set up a new Calibration
For Help, press F1
Status
10:24 AM
5/1/18


ApplicationWizard
File
View
Options
Help
New Application... Ctrl+N
Open Application... Ctrl+I
Draft Application... Ctrl+U
Open Compound Library
Setup mode
Print Setup...
1 Obsidian.evm
2 Mudrock Trace Green.evm
3 Mudrock Trace Green.devm
Exit
Click *File* and then *New Application*
Create a new Application
Status
10:24 AM
5/1/18


ApplicationWizard
File View Options Help
Give your new calibration a name. Don’t worry about normalizations - we will handle those later
New Application
New application name:
Obsidian
Time based empirical
Compton based empirical
Sum ROI based empirical
OK
Cancel
For Help, press F1
Status
10:25 AM
5/1/18

ApplicationWizard - [Obsidian.devm *]

File Edit View Method Calibration Window Options Help

Obsidian
- Materials
- Measurement
- Calibration
- Modules
- Application

Please push "Next" button

EasyCal ApplicationWizard Program

ApplicationWizard makes it possible to define an XRF Application through a succession of steps, while providing manual adjustments and flexibility at all steps to meet complex specific demands.

To create a XRF application, just follow the steps presented in the left explorer pane one by one, and save the document. The complete procedure creates an Application file (name.evm) which contains references to the method files of the application, together with various options which can be selected at the last step of the process (the Application step). In addition an installation package is created, with the <name>.calibration, <name>.aen and <name>.xrd files, which can be installed using BIT.

Opening a Spectra^{EDX}/EasyCal Application file:

Use the File | New command, select the nam,e for the new application and follow the steps. A new Application starts out as a Draft Application (DEVM file). This Draft Application will be converted to a working Application (EVM file) in the last step (the Application step).

Creating a new application from scratch:

Use the File | New command, select the name for the new application and follow the steps. A new Application starts out as a Draft Applications (DEVM file). This Draft Application will be converted to working Application (EVM file) in the last step (the Application step).

Materials | Compounds step):

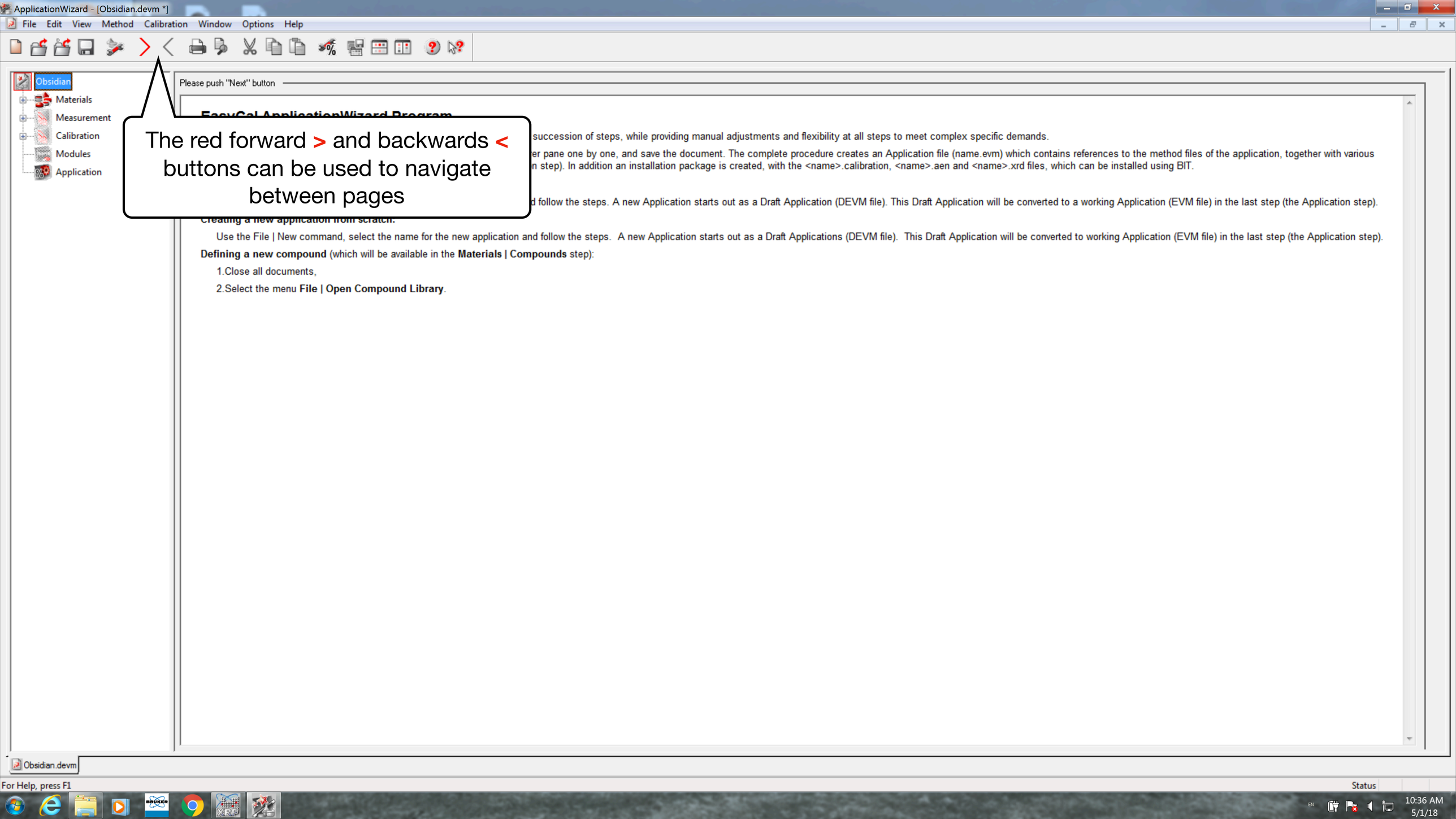
Your calibration will commence in a linear process using the side panel

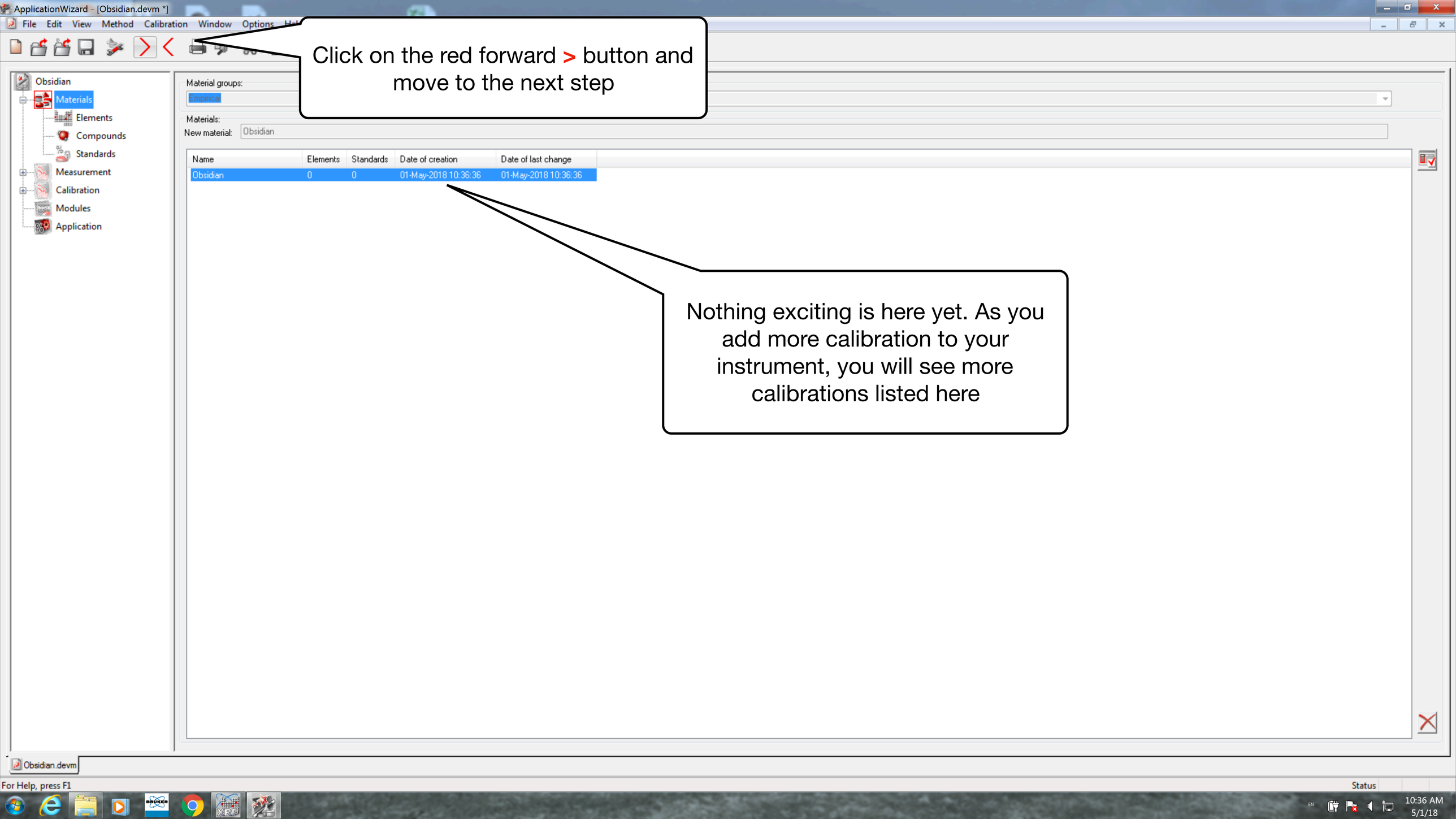
Obsidian.devm

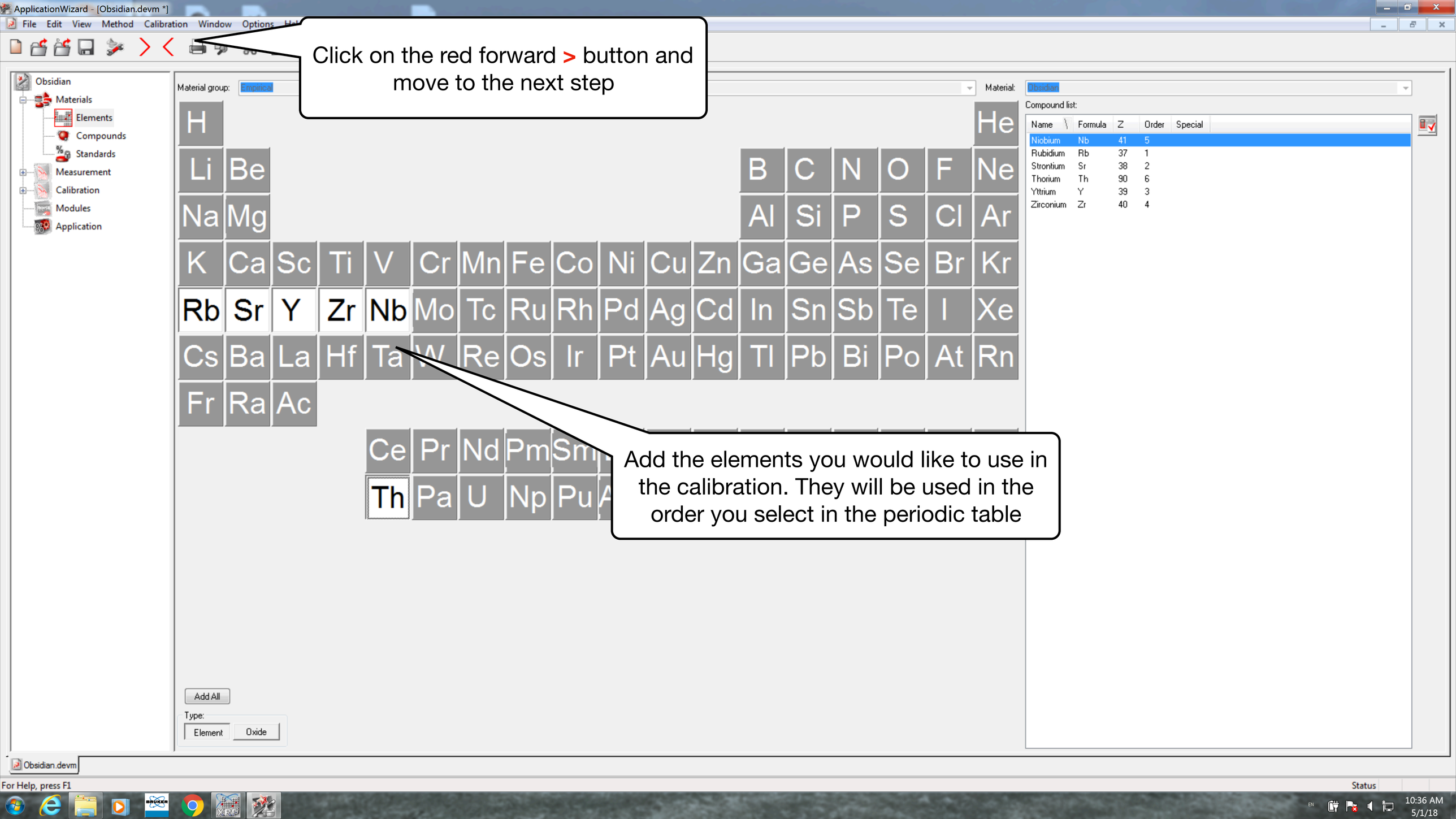
For Help, press F1

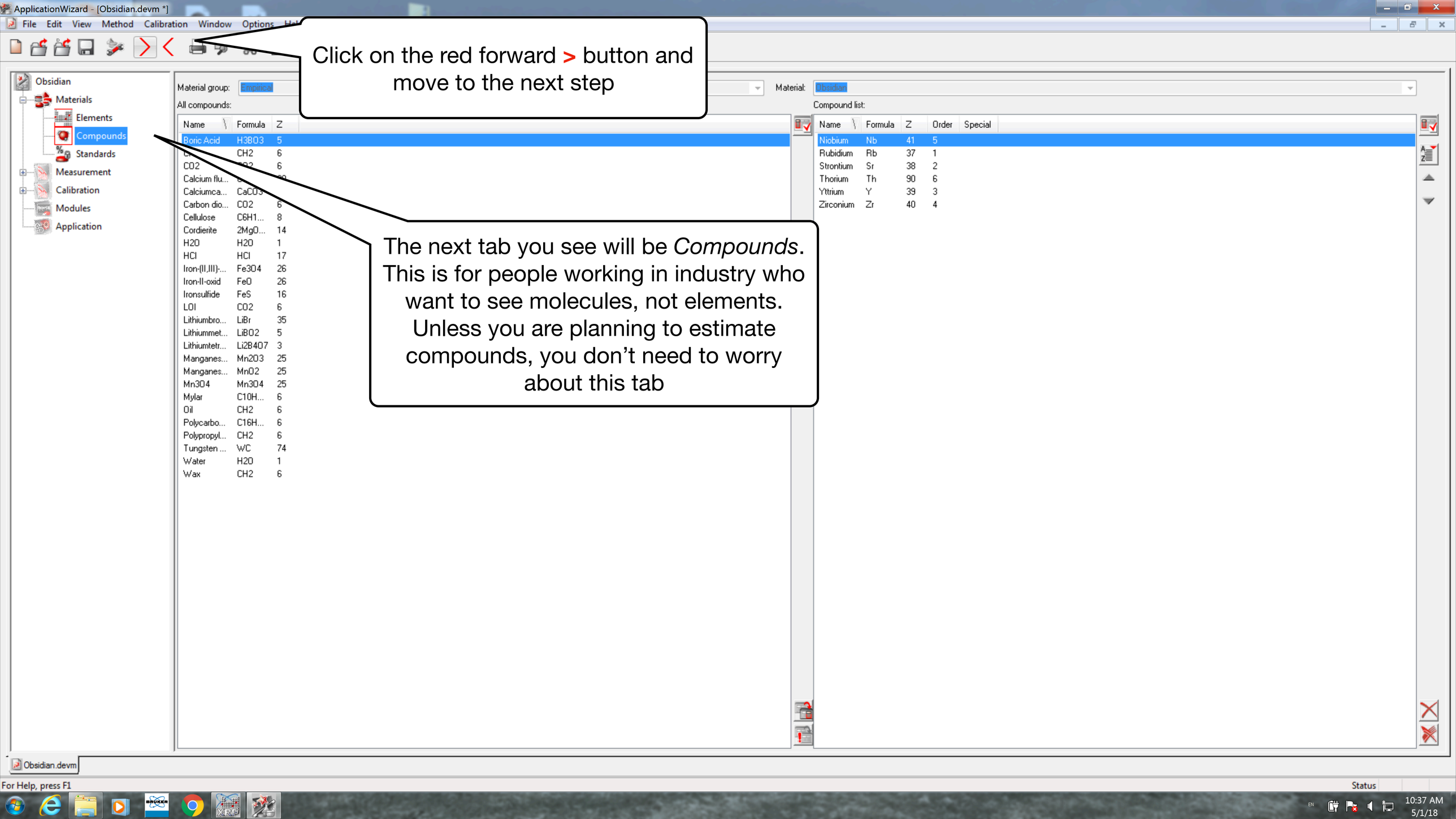
Status

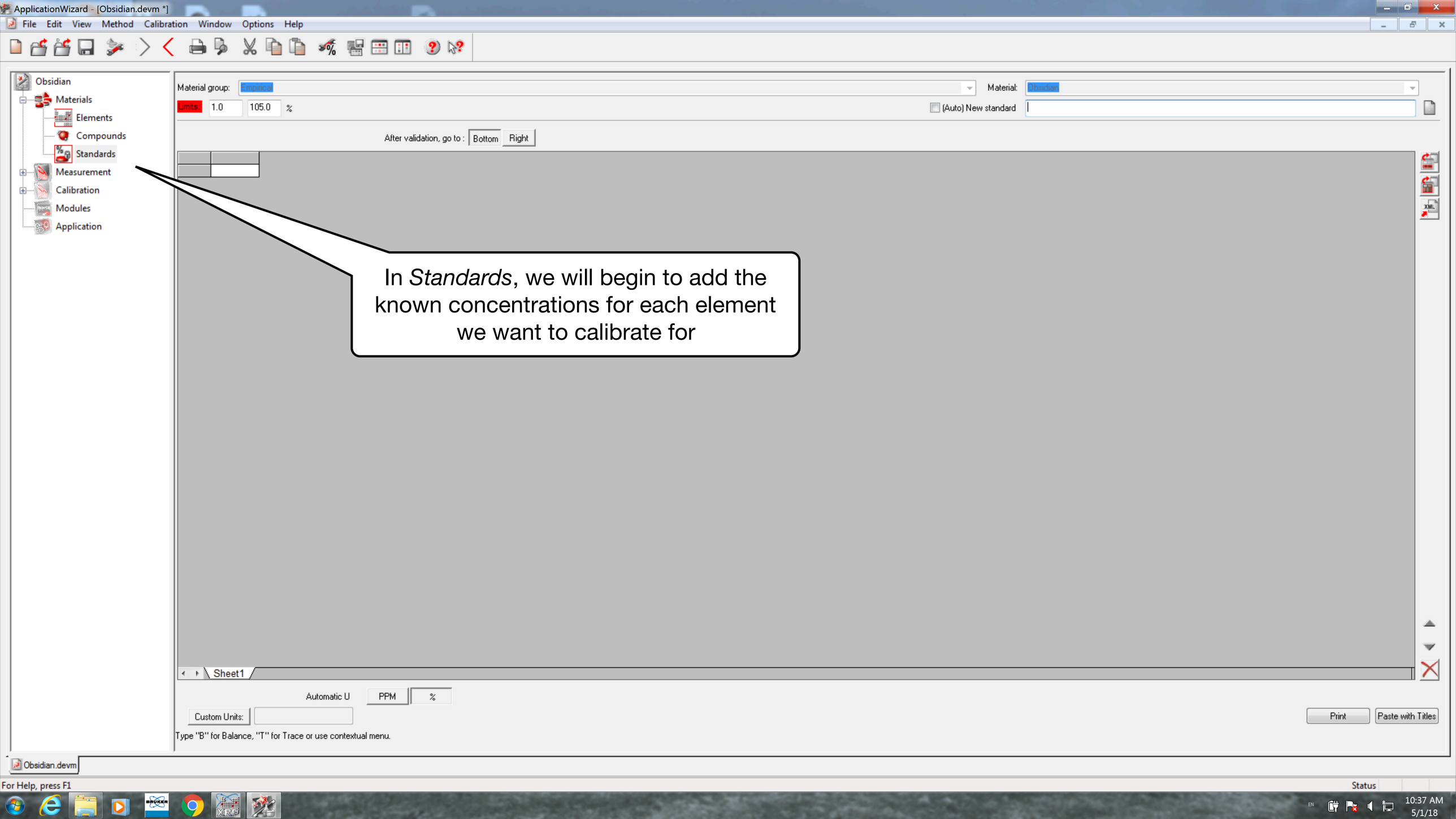
10:36 AM
5/1/18

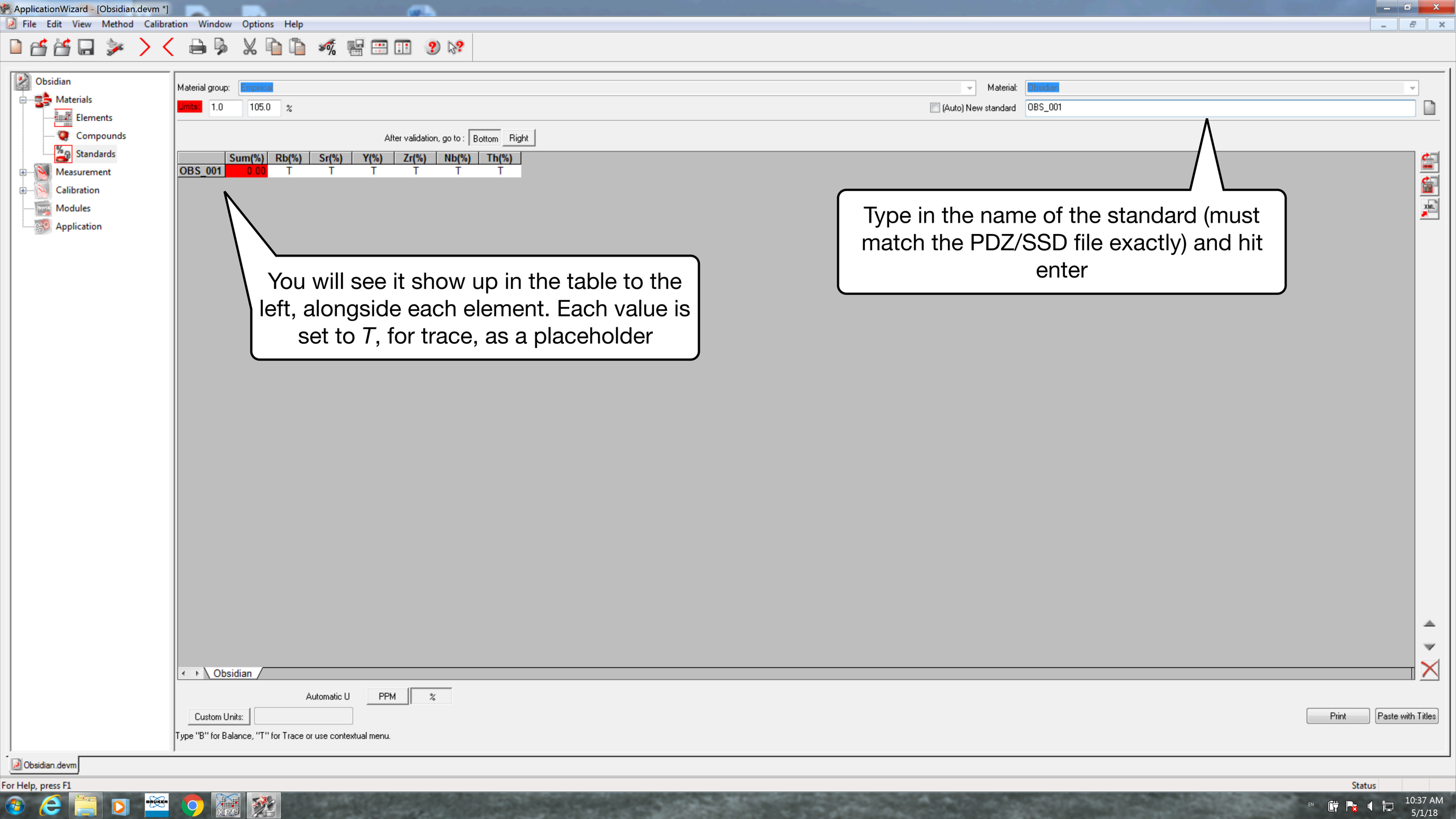

ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Obsidian
Materials
Measurement
Calibration
Modules
Application
The red forward > and backwards < buttons can be used to navigate between pages
Please push "Next" button
succession of steps, while providing manual adjustments and flexibility at all steps to meet complex specific demands.
er pane one by one, and save the document. The complete procedure creates an Application file (name.evm) which contains references to the method files of the application, together with various
n step). In addition an installation package is created, with the <name>.calibration, <name>.aen and <name>.xrd files, which can be installed using BIT.
d follow the steps. A new Application starts out as a Draft Application (DEVM file). This Draft Application will be converted to a working Application (EVM file) in the last step (the Application step).
Creating a new application from scratch:
Use the File | New command, select the name for the new application and follow the steps. A new Application starts out as a Draft Applications (DEVM file). This Draft Application will be converted to working Application (EVM file) in the last step (the Application step).
Defining a new compound (which will be available in the Materials | Compounds step):
1.Close all documents,
2.Select the menu File | Open Compound Library.
Obsidian.devm
For Help, press F1
Status
10:36 AM
5/1/18

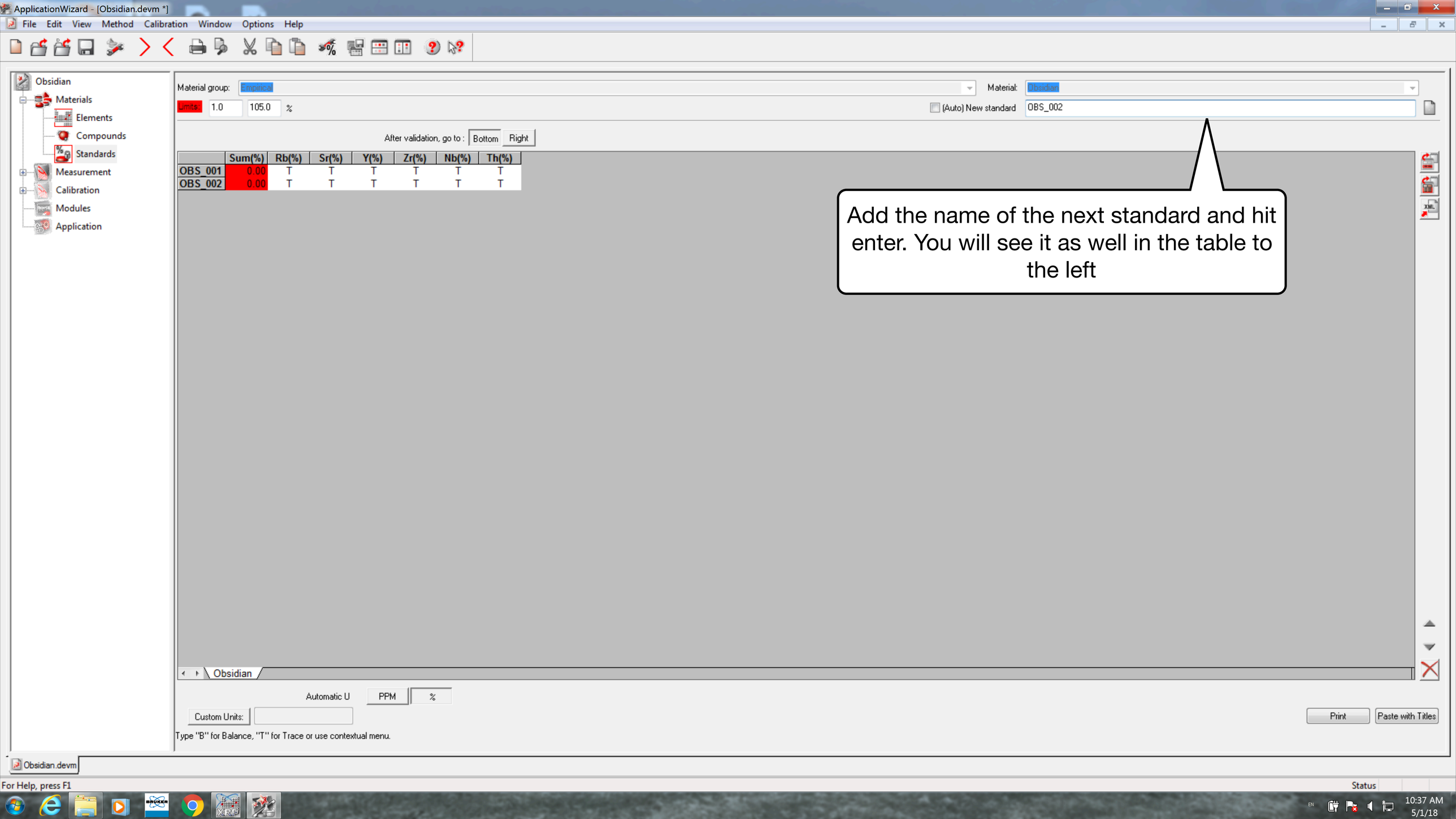

ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Click on the red forward > button and move to the next step
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material groups:
Empirical
Materials:
New material:
Obsidian
Name
Elements
Standards
Date of creation
Date of last change
Obsidian
0
0
01-May-2018 10:36:36
01-May-2018 10:36:36
Nothing exciting is here yet. As you add more calibration to your instrument, you will see more calibrations listed here
Obsidian.devm
For Help, press F1
Status
10:36 AM
5/1/18

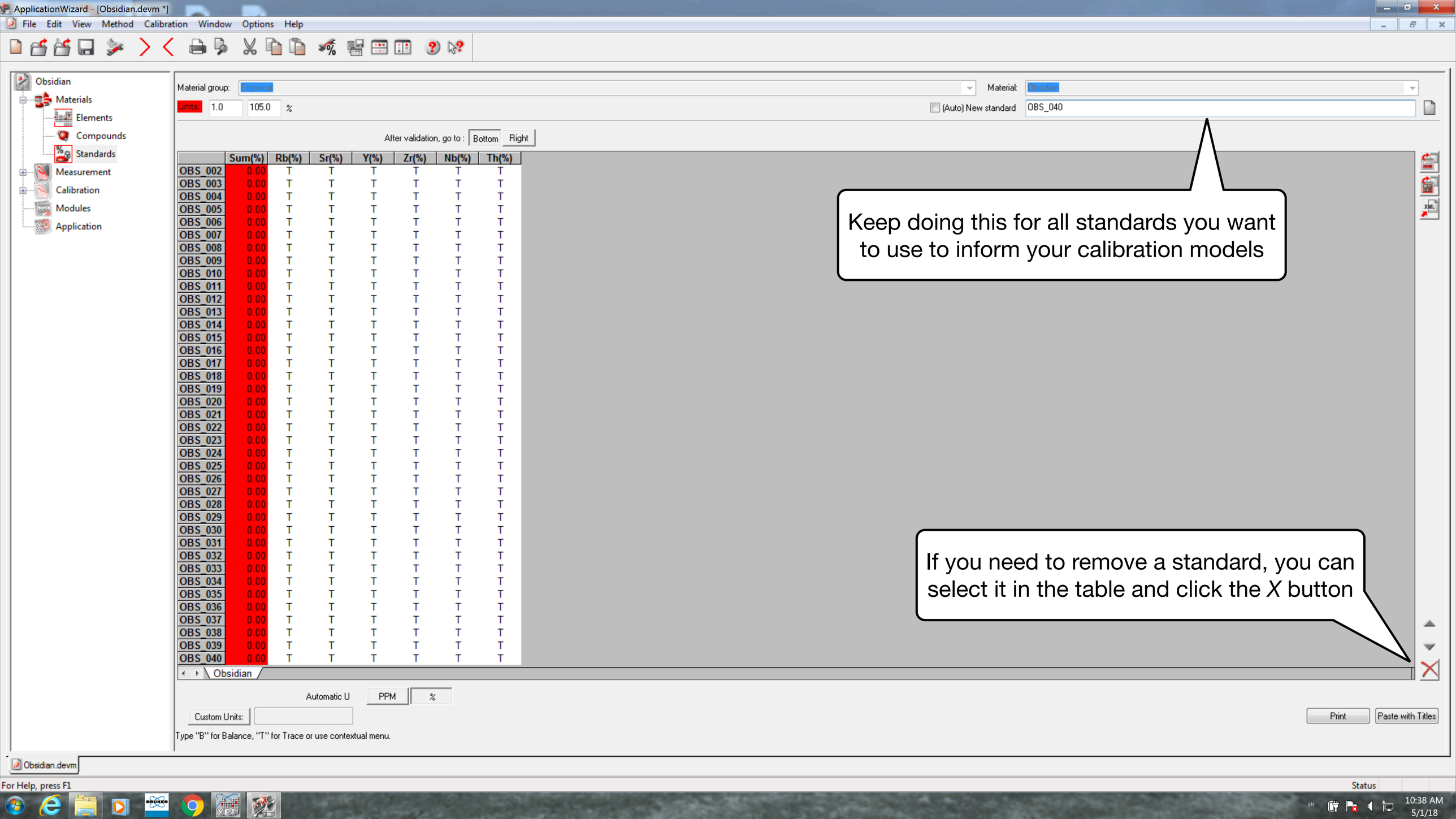

ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Click on the red forward > button and move to the next step
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material group: Empirical
Material: Obsidian
Compound list:
Name Formula Z Order Special
Niobium Nb 41 5
Rubidium Rb 37 1
Strontium Sr 38 2
Thorium Th 90 6
Yttrium Y 39 3
Zirconium Zr 40 4
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
Fr Ra Ac
Ce Pr Nd Pm Sm
Th Pa U Np Pu
Add the elements you would like to use in the calibration. They will be used in the order you select in the periodic table
Add All
Type:
Element
Oxide
Obsidian.devm
For Help, press F1
Status
10:36 AM
5/1/18

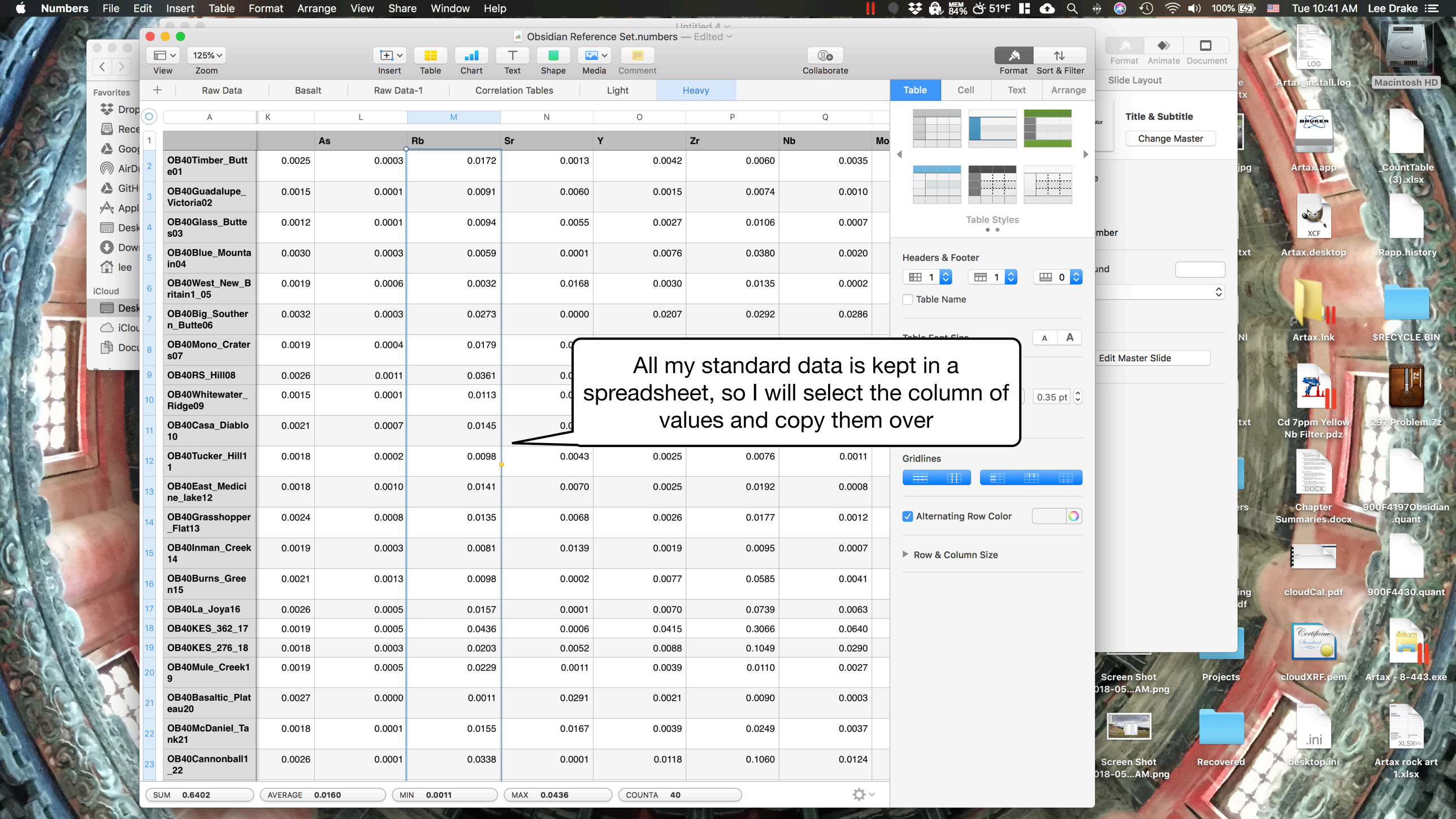

ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options
Click on the red forward > button and move to the next step
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material group: Empirical
Material: Obsidian
All compounds:
Compound list:
Name Formula Z
Boric Acid H3BO3 5
CH2 6
CO2 6
Calcium flu...
Calciumca... CaCO3
Carbon dio... CO2 6
Cellulose C6H1... 8
Cordierite 2MgO... 14
H2O H2O 1
HCl HCl 17
Iron-(II,III)-... Fe3O4 26
Iron-II-oxid FeO 26
Ironsulfide FeS 16
LOI CO2 6
Lithiumbro... LiBr 35
Lithiummet... LiBO2 5
Lithiumtetr... Li2B4O7 3
Manganes... Mn2O3 25
Manganes... MnO2 25
Mn3O4 Mn3O4 25
Mylar C10H... 6
Oil CH2 6
Polycarbo... C16H... 6
Polypropyl... CH2 6
Tungsten ... WC 74
Water H2O 1
Wax CH2 6
Name Formula Z Order Special
Niobium Nb 41 5
Rubidium Rb 37 1
Strontium Sr 38 2
Thorium Th 90 6
Yttrium Y 39 3
Zirconium Zr 40 4
The next tab you see will be Compounds. This is for people working in industry who want to see molecules, not elements. Unless you are planning to estimate compounds, you don't need to worry about this tab
Obsidian.devm
For Help, press F1
Status
10:37 AM
5/1/18


ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material group: Empirical
Material: Obsidian
Limits: 1.0 105.0 %
(Auto) New standard
After validation, go to : Bottom Right
In Standards, we will begin to add the known concentrations for each element we want to calibrate for
Sheet1
Automatic U PPM %
Custom Units:
Print Paste with Titles
Type "B" for Balance, "T" for Trace or use contextual menu.
Obsidian.devm
For Help, press F1
Status
10:37 AM
5/1/18


ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material group: Empirical
Material: Obsidian
Limits: 1.0 105.0 %
(Auto) New standard
OBS_001
After validation, go to : Bottom Right
Sum(%) Rb(%) Sr(%) Y(%) Zr(%) Nb(%) Th(%)
OBS_001 0.00 T T T T T T
You will see it show up in the table to the left, alongside each element. Each value is set to T, for trace, as a placeholder
Type in the name of the standard (must match the PDZ/SSD file exactly) and hit enter
Obsidian
Automatic U
PPM
%
Custom Units:
Print
Paste with Titles
Type "B" for Balance, "T" for Trace or use contextual menu.
Obsidian.devm
For Help, press F1
Status
10:37 AM
5/1/18

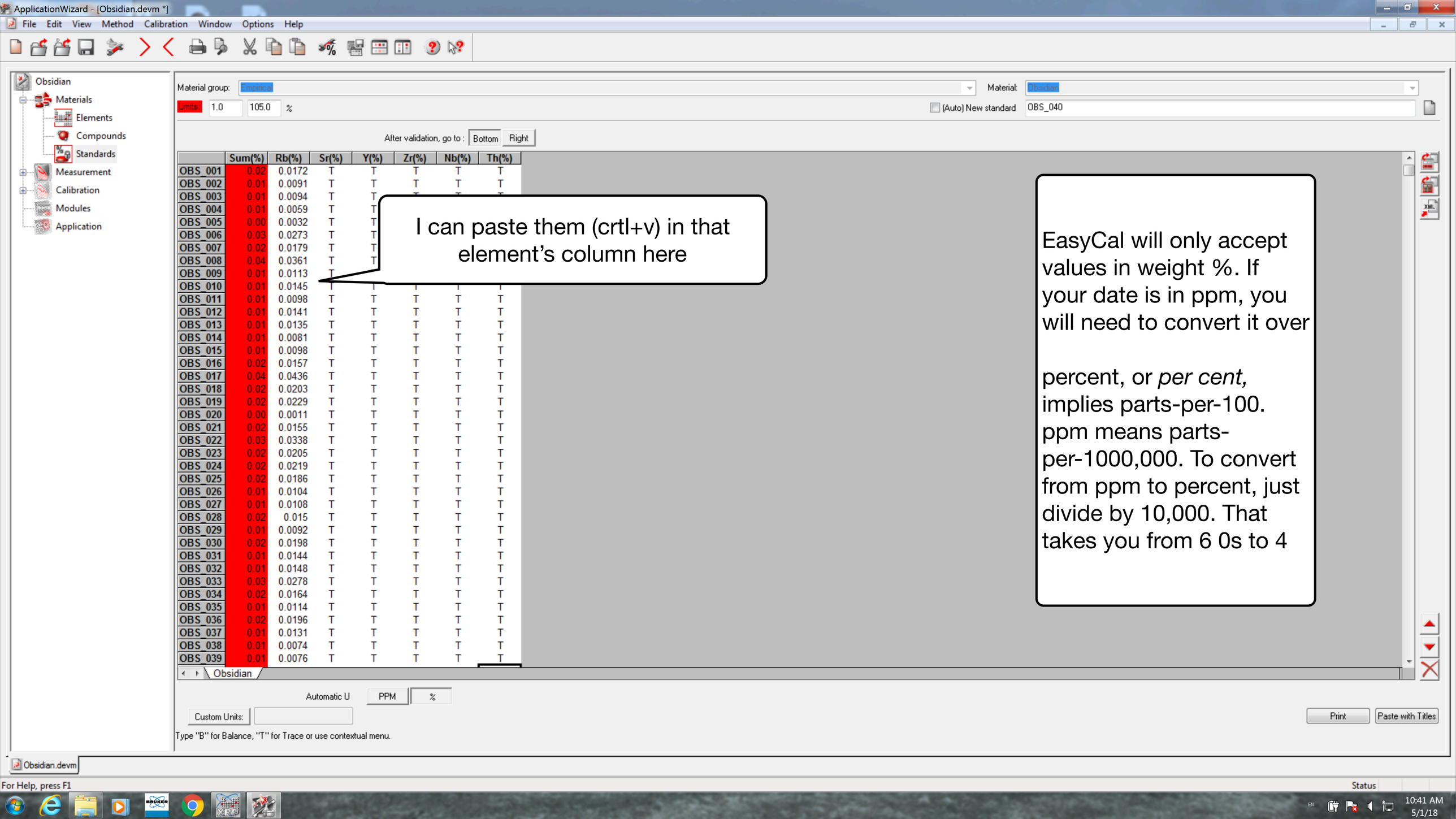

ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material group: Empirical
Material: Obsidian
Limits: 1.0 105.0 %
(Auto) New standard
OBS_002
After validation, go to : Bottom Right
Sum(%) Rb(%) Sr(%) Y(%) Zr(%) Nb(%) Th(%)
OBS_001 0.00 T T T T T T
OBS_002 0.00 T T T T T T
Add the name of the next standard and hit enter. You will see it as well in the table to the left
Obsidian
Automatic U
PPM
%
Custom Units:
Print
Paste with Titles
Type "B" for Balance, "T" for Trace or use contextual menu.
Obsidian.devm
For Help, press F1
Status
10:37 AM
5/1/18

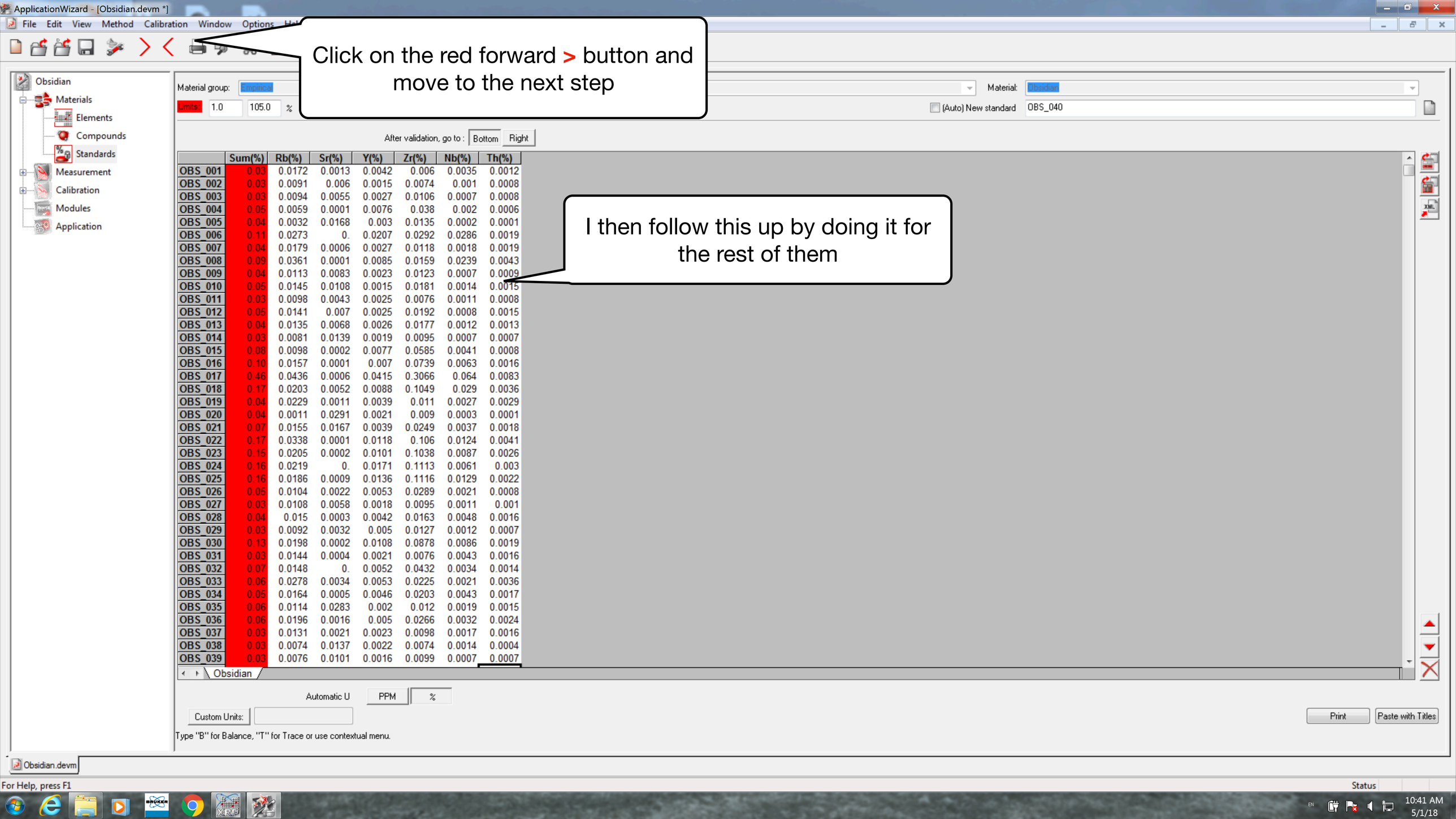

ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material group: Empirical
Material: Obsidian
Limits: 1.0 105.0 %
(Auto) New standard
OBS_040
After validation, go to : Bottom Right
Sum(%) Rb(%) Sr(%) Y(%) Zr(%) Nb(%) Th(%)
OBS_002 0.00 T T T T T T
OBS_003 0.00 T T T T T T
OBS_004 0.00 T T T T T T
OBS_005 0.00 T T T T T T
OBS_006 0.00 T T T T T T
OBS_007 0.00 T T T T T T
OBS_008 0.00 T T T T T T
OBS_009 0.00 T T T T T T
OBS_010 0.00 T T T T T T
OBS_011 0.00 T T T T T T
OBS_012 0.00 T T T T T T
OBS_013 0.00 T T T T T T
OBS_014 0.00 T T T T T T
OBS_015 0.00 T T T T T T
OBS_016 0.00 T T T T T T
OBS_017 0.00 T T T T T T
OBS_018 0.00 T T T T T T
OBS_019 0.00 T T T T T T
OBS_020 0.00 T T T T T T
OBS_021 0.00 T T T T T T
OBS_022 0.00 T T T T T T
OBS_023 0.00 T T T T T T
OBS_024 0.00 T T T T T T
OBS_025 0.00 T T T T T T
OBS_026 0.00 T T T T T T
OBS_027 0.00 T T T T T T
OBS_028 0.00 T T T T T T
OBS_029 0.00 T T T T T T
OBS_030 0.00 T T T T T T
OBS_031 0.00 T T T T T T
OBS_032 0.00 T T T T T T
OBS_033 0.00 T T T T T T
OBS_034 0.00 T T T T T T
OBS_035 0.00 T T T T T T
OBS_036 0.00 T T T T T T
OBS_037 0.00 T T T T T T
OBS_038 0.00 T T T T T T
OBS_039 0.00 T T T T T T
OBS_040 0.00 T T T T T T
Obsidian
Automatic U
PPM
%
Custom Units:
Type "B" for Balance, "T" for Trace or use contextual menu.
Print
Paste with Titles
Keep doing this for all standards you want to use to inform your calibration models
If you need to remove a standard, you can select it in the table and click the X button
Obsidian.devm
For Help, press F1
Status
10:38 AM
5/1/18



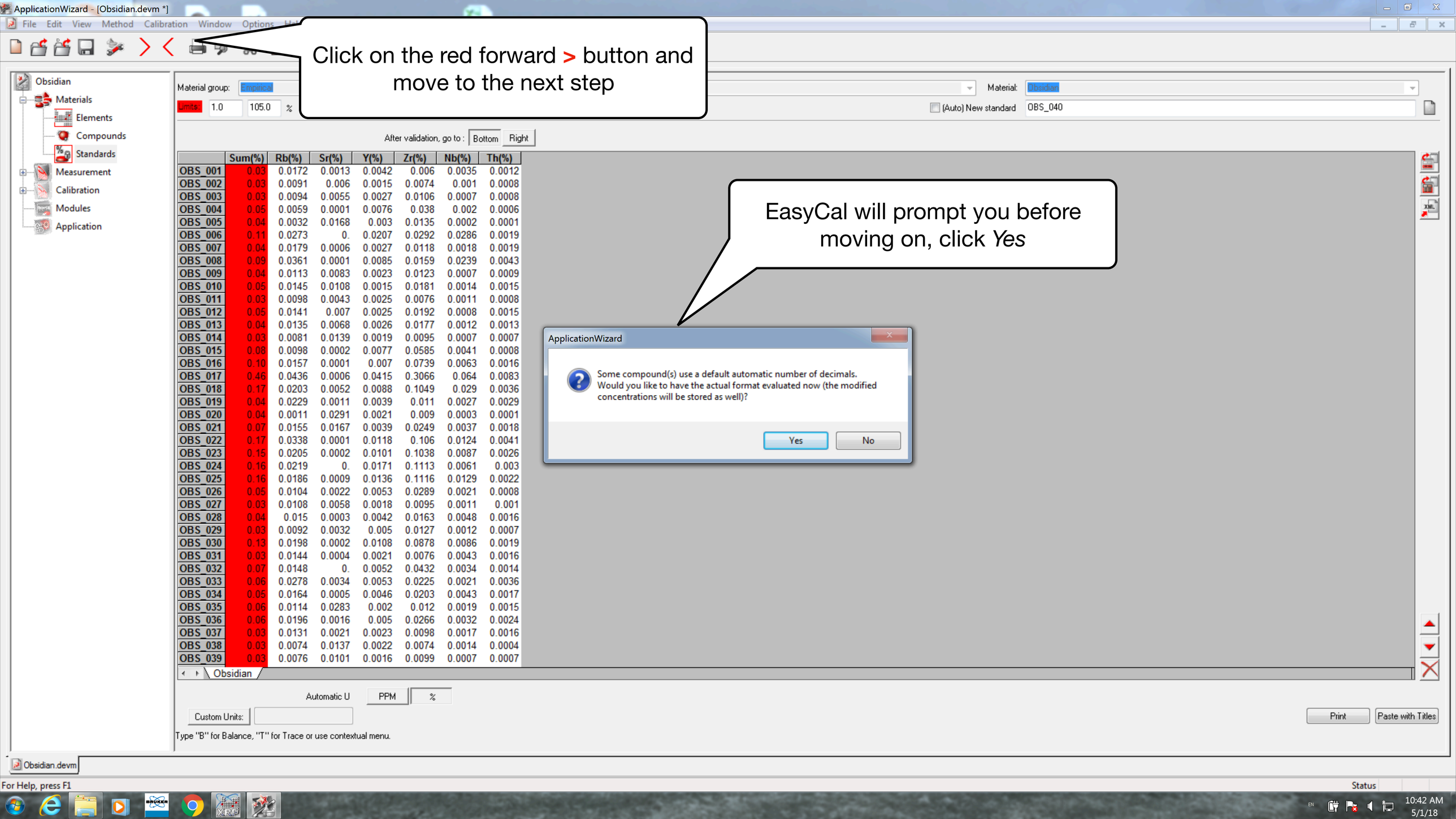
		As	Rb	Sr	Y	Zr	Nb	Mo
OB40Timber_Butte01	0.0025	0.0003	0.0172	0.0013	0.0042	0.0060	0.0035	
OB40Guadalupe_Victoria02	0.0015	0.0001	0.0091	0.0060	0.0015	0.0074	0.0010	
OB40Glass_Buttes03	0.0012	0.0001	0.0094	0.0055	0.0027	0.0106	0.0007	
OB40Blue_Mountain04	0.0030	0.0003	0.0059	0.0001	0.0076	0.0380	0.0020	
OB40West_New_Britain1_05	0.0019	0.0006	0.0032	0.0168	0.0030	0.0135	0.0002	
OB40Big_Southern_Butte06	0.0032	0.0003	0.0273	0.0000	0.0207	0.0292	0.0286	
OB40Mono_Craters07	0.0019	0.0004	0.0179	0.0				
OB40RS_Hill08	0.0026	0.0011	0.0361	0.0				
OB40Whitewater_Ridge09	0.0015	0.0001	0.0113	0.0				
OB40Casa_Diablo10	0.0021	0.0007	0.0145	0.0				
OB40Tucker_Hill11	0.0018	0.0002	0.0098	0.0043	0.0025	0.0076	0.0011	
OB40East_Medicine_lake12	0.0018	0.0010	0.0141	0.0070	0.0025	0.0192	0.0008	
OB40Grasshopper_Flat13	0.0024	0.0008	0.0135	0.0068	0.0026	0.0177	0.0012	
OB40Inman_Creek14	0.0019	0.0003	0.0081	0.0139	0.0019	0.0095	0.0007	
OB40Burns_Green15	0.0021	0.0013	0.0098	0.0002	0.0077	0.0585	0.0041	
OB40La_Joya16	0.0026	0.0005	0.0157	0.0001	0.0070	0.0739	0.0063	
OB40KES_362_17	0.0019	0.0005	0.0436	0.0006	0.0415	0.3066	0.0640	
OB40KES_276_18	0.0018	0.0003	0.0203	0.0052	0.0088	0.1049	0.0290	
OB40Mule_Creek19	0.0019	0.0005	0.0229	0.0011	0.0039	0.0110	0.0027	
OB40Basaltic_Plateau20	0.0027	0.0000	0.0011	0.0291	0.0021	0.0090	0.0003	
OB40McDaniel_Tank21	0.0018	0.0001	0.0155	0.0167	0.0039	0.0249	0.0037	
OB40Cannonball1_22	0.0026	0.0001	0.0338	0.0001	0.0118	0.1060	0.0124	

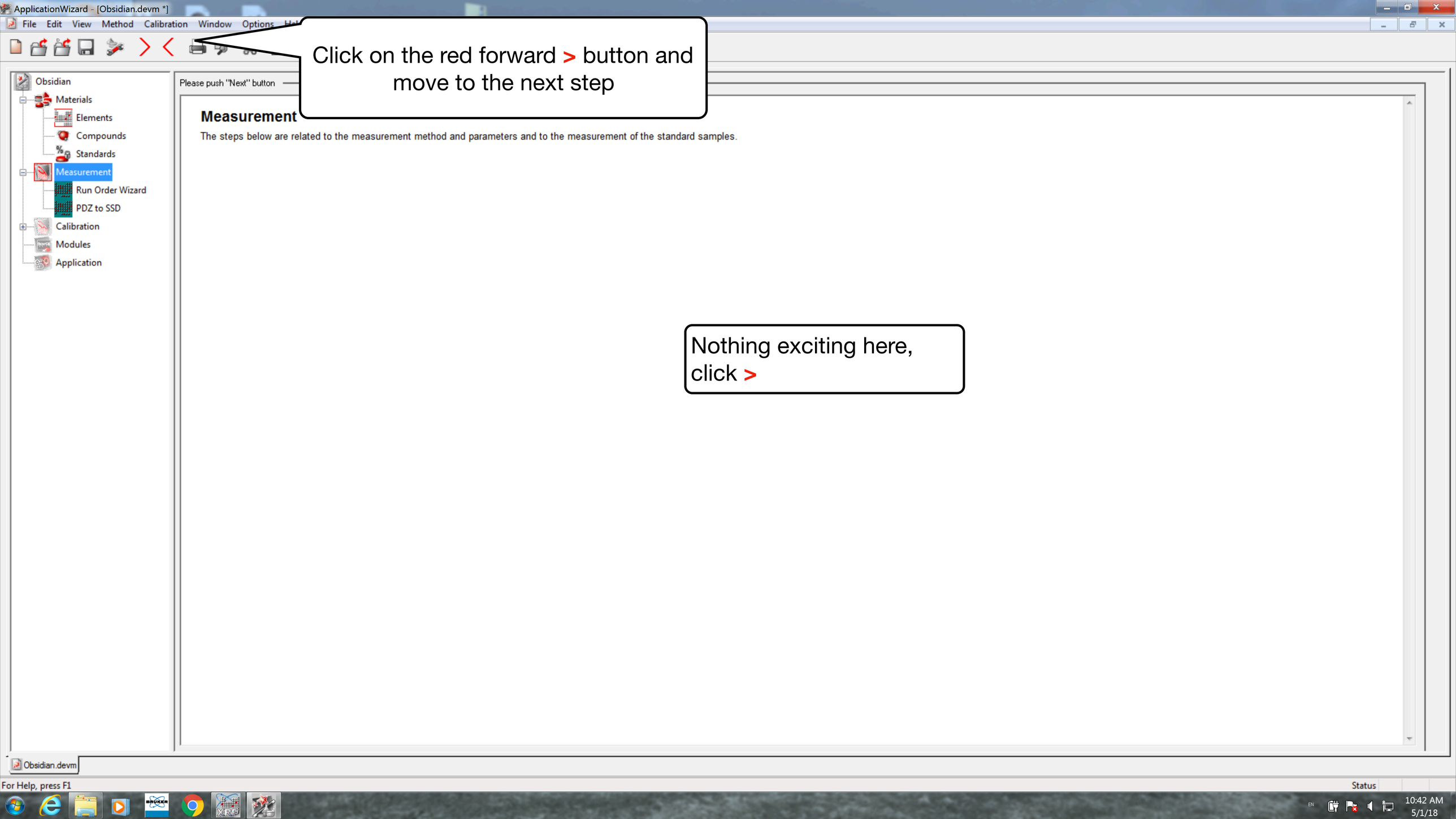
SUM 0.6402 | AVERAGE 0.0160 | MIN 0.0011 | MAX 0.0436 | COUNTA 40


ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material group: Empirical
Material: Obsidian
Limits: 1.0 105.0 %
(Auto) New standard OBS_040
After validation, go to : Bottom Right
Sum(%) Rb(%) Sr(%) Y(%) Zr(%) Nb(%) Th(%)
OBS_001 0.02 0.0172 T T T T T
OBS_002 0.01 0.0091 T T T T T
OBS_003 0.01 0.0094 T T
OBS_004 0.01 0.0059 T T
OBS_005 0.00 0.0032 T T
OBS_006 0.03 0.0273 T T
OBS_007 0.02 0.0179 T T
OBS_008 0.04 0.0361 T T
OBS_009 0.01 0.0113 T
OBS_010 0.01 0.0145
OBS_011 0.01 0.0098 T T T T T
OBS_012 0.01 0.0141 T T T T T
OBS_013 0.01 0.0135 T T T T T
OBS_014 0.01 0.0081 T T T T T
OBS_015 0.01 0.0098 T T T T T
OBS_016 0.02 0.0157 T T T T T
OBS_017 0.04 0.0436 T T T T T
OBS_018 0.02 0.0203 T T T T T
OBS_019 0.02 0.0229 T T T T T
OBS_020 0.00 0.0011 T T T T T
OBS_021 0.02 0.0155 T T T T T
OBS_022 0.03 0.0338 T T T T T
OBS_023 0.02 0.0205 T T T T T
OBS_024 0.02 0.0219 T T T T T
OBS_025 0.02 0.0186 T T T T T
OBS_026 0.01 0.0104 T T T T T
OBS_027 0.01 0.0108 T T T T T
OBS_028 0.02 0.015 T T T T T
OBS_029 0.01 0.0092 T T T T T
OBS_030 0.02 0.0198 T T T T T
OBS_031 0.01 0.0144 T T T T T
OBS_032 0.01 0.0148 T T T T T
OBS_033 0.03 0.0278 T T T T T
OBS_034 0.02 0.0164 T T T T T
OBS_035 0.01 0.0114 T T T T T
OBS_036 0.02 0.0196 T T T T T
OBS_037 0.01 0.0131 T T T T T
OBS_038 0.01 0.0074 T T T T T
OBS_039 0.01 0.0076 T T T T T
Obsidian
I can paste them (crtl+v) in that element's column here
EasyCal will only accept values in weight %. If your date is in ppm, you will need to convert it over
percent, or per cent, implies parts-per-100. ppm means parts-per-1000,000. To convert from ppm to percent, just divide by 10,000. That takes you from 6 0s to 4
Automatic U PPM %
Custom Units:
Type "B" for Balance, "T" for Trace or use contextual menu.
Print Paste with Titles
Obsidian.devm
For Help, press F1
Status
10:41 AM
5/1/18



	Sum(%)	Rb(%)	Sr(%)	Y(%)	Zr(%)	Nb(%)	Th(%)
OBS_001	0.03	0.0172	0.0013	0.0042	0.006	0.0035	0.0012
OBS_002	0.03	0.0091	0.006	0.0015	0.0074	0.001	0.0008
OBS_003	0.03	0.0094	0.0055	0.0027	0.0106	0.0007	0.0008
OBS_004	0.05	0.0059	0.0001	0.0076	0.038	0.002	0.0006
OBS_005	0.04	0.0032	0.0168	0.003	0.0135	0.0002	0.0001
OBS_006	0.11	0.0273	0.	0.0207	0.0292	0.0286	0.0019
OBS_007	0.04	0.0179	0.0006	0.0027	0.0118	0.0018	0.0019
OBS_008	0.09	0.0361	0.0001	0.0085	0.0159	0.0239	0.0043
OBS_009	0.04	0.0113	0.0083	0.0023	0.0123	0.0007	0.0009
OBS_010	0.05	0.0145	0.0108	0.0015	0.0181	0.0014	0.0015
OBS_011	0.03	0.0098	0.0043	0.0025	0.0076	0.0011	0.0008
OBS_012	0.05	0.0141	0.007	0.0025	0.0192	0.0008	0.0015
OBS_013	0.04	0.0135	0.0068	0.0026	0.0177	0.0012	0.0013
OBS_014	0.03	0.0081	0.0139	0.0019	0.0095	0.0007	0.0007
OBS_015	0.08	0.0098	0.0002	0.0077	0.0585	0.0041	0.0008
OBS_016	0.10	0.0157	0.0001	0.007	0.0739	0.0063	0.0016
OBS_017	0.46	0.0436	0.0006	0.0415	0.3066	0.064	0.0083
OBS_018	0.17	0.0203	0.0052	0.0088	0.1049	0.029	0.0036
OBS_019	0.04	0.0229	0.0011	0.0039	0.011	0.0027	0.0029
OBS_020	0.04	0.0011	0.0291	0.0021	0.009	0.0003	0.0001
OBS_021	0.07	0.0155	0.0167	0.0039	0.0249	0.0037	0.0018
OBS_022	0.17	0.0338	0.0001	0.0118	0.106	0.0124	0.0041
OBS_023	0.15	0.0205	0.0002	0.0101	0.1038	0.0087	0.0026
OBS_024	0.16	0.0219	0.	0.0171	0.1113	0.0061	0.003
OBS_025	0.16	0.0186	0.0009	0.0136	0.1116	0.0129	0.0022
OBS_026	0.05	0.0104	0.0022	0.0053	0.0289	0.0021	0.0008
OBS_027	0.03	0.0108	0.0058	0.0018	0.0095	0.0011	0.001
OBS_028	0.04	0.015	0.0003	0.0042	0.0163	0.0048	0.0016
OBS_029	0.03	0.0092	0.0032	0.005	0.0127	0.0012	0.0007
OBS_030	0.13	0.0198	0.0002	0.0108	0.0878	0.0086	0.0019
OBS_031	0.03	0.0144	0.0004	0.0021	0.0076	0.0043	0.0016
OBS_032	0.07	0.0148	0.	0.0052	0.0432	0.0034	0.0014
OBS_033	0.06	0.0278	0.0034	0.0053	0.0225	0.0021	0.0036
OBS_034	0.05	0.0164	0.0005	0.0046	0.0203	0.0043	0.0017
OBS_035	0.06	0.0114	0.0283	0.002	0.012	0.0019	0.0015
OBS_036	0.06	0.0196	0.0016	0.005	0.0266	0.0032	0.0024
OBS_037	0.03	0.0131	0.0021	0.0023	0.0098	0.0017	0.0016
OBS_038	0.03	0.0074	0.0137	0.0022	0.0074	0.0014	0.0004
OBS_039	0.03	0.0076	0.0101	0.0016	0.0099	0.0007	0.0007


ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options
Click on the red forward > button and move to the next step
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Calibration
Modules
Application
Material group: Empirical
Material: Obsidian
Limits: 1.0 105.0 %
(Auto) New standard OBS_040
After validation, go to : Bottom Right
Sum(%) Rb(%) Sr(%) Y(%) Zr(%) Nb(%) Th(%)
OBS_001 0.03 0.0172 0.0013 0.0042 0.006 0.0035 0.0012
OBS_002 0.03 0.0091 0.006 0.0015 0.0074 0.001 0.0008
OBS_003 0.03 0.0094 0.0055 0.0027 0.0106 0.0007 0.0008
OBS_004 0.05 0.0059 0.0001 0.0076 0.038 0.002 0.0006
OBS_005 0.04 0.0032 0.0168 0.003 0.0135 0.0002 0.0001
OBS_006 0.11 0.0273 0. 0.0207 0.0292 0.0286 0.0019
OBS_007 0.04 0.0179 0.0006 0.0027 0.0118 0.0018 0.0019
OBS_008 0.09 0.0361 0.0001 0.0085 0.0159 0.0239 0.0043
OBS_009 0.04 0.0113 0.0083 0.0023 0.0123 0.0007 0.0009
OBS_010 0.05 0.0145 0.0108 0.0015 0.0181 0.0014 0.0015
OBS_011 0.03 0.0098 0.0043 0.0025 0.0076 0.0011 0.0008
OBS_012 0.05 0.0141 0.007 0.0025 0.0192 0.0008 0.0015
OBS_013 0.04 0.0135 0.0068 0.0026 0.0177 0.0012 0.0013
OBS_014 0.03 0.0081 0.0139 0.0019 0.0095 0.0007 0.0007
OBS_015 0.08 0.0098 0.0002 0.0077 0.0585 0.0041 0.0008
OBS_016 0.10 0.0157 0.0001 0.007 0.0739 0.0063 0.0016
OBS_017 0.46 0.0436 0.0006 0.0415 0.3066 0.064 0.0083
OBS_018 0.17 0.0203 0.0052 0.0088 0.1049 0.029 0.0036
OBS_019 0.04 0.0229 0.0011 0.0039 0.011 0.0027 0.0029
OBS_020 0.04 0.0011 0.0291 0.0021 0.009 0.0003 0.0001
OBS_021 0.07 0.0155 0.0167 0.0039 0.0249 0.0037 0.0018
OBS_022 0.17 0.0338 0.0001 0.0118 0.106 0.0124 0.0041
OBS_023 0.15 0.0205 0.0002 0.0101 0.1038 0.0087 0.0026
OBS_024 0.16 0.0219 0. 0.0171 0.1113 0.0061 0.003
OBS_025 0.16 0.0186 0.0009 0.0136 0.1116 0.0129 0.0022
OBS_026 0.05 0.0104 0.0022 0.0053 0.0289 0.0021 0.0008
OBS_027 0.03 0.0108 0.0058 0.0018 0.0095 0.0011 0.001
OBS_028 0.04 0.015 0.0003 0.0042 0.0163 0.0048 0.0016
OBS_029 0.03 0.0092 0.0032 0.005 0.0127 0.0012 0.0007
OBS_030 0.13 0.0198 0.0002 0.0108 0.0878 0.0086 0.0019
OBS_031 0.03 0.0144 0.0004 0.0021 0.0076 0.0043 0.0016
OBS_032 0.07 0.0148 0. 0.0052 0.0432 0.0034 0.0014
OBS_033 0.06 0.0278 0.0034 0.0053 0.0225 0.0021 0.0036
OBS_034 0.05 0.0164 0.0005 0.0046 0.0203 0.0043 0.0017
OBS_035 0.06 0.0114 0.0283 0.002 0.012 0.0019 0.0015
OBS_036 0.06 0.0196 0.0016 0.005 0.0266 0.0032 0.0024
OBS_037 0.03 0.0131 0.0021 0.0023 0.0098 0.0017 0.0016
OBS_038 0.03 0.0074 0.0137 0.0022 0.0074 0.0014 0.0004
OBS_039 0.03 0.0076 0.0101 0.0016 0.0099 0.0007 0.0007
Obsidian
EasyCal will prompt you before moving on, click Yes
ApplicationWizard
Some compound(s) use a default automatic number of decimals.
Would you like to have the actual format evaluated now (the modified concentrations will be stored as well)?
Yes
No
Automatic U PPM %
Custom Units:
Print Paste with Titles
Type "B" for Balance, "T" for Trace or use contextual menu.
Obsidian.devm
For Help, press F1
Status
10:42 AM
5/1/18


ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Click on the red forward > button and move to the next step
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Modules
Application
Please push "Next" button
Measurement
The steps below are related to the measurement method and parameters and to the measurement of the standard samples.
Nothing exciting here, click >
Obsidian.devm
For Help, press F1
Status
10:42 AM
5/1/18

ApplicationWizard - [Obsidian.devm *]

File Edit View Method Calibration Window Options Help

Obsidian
- Materials
  - Elements
  - Compounds
  - Standards
- Measurement
  - Run Order Wizard
  - PDZ to SSD
- Calibration
- Modules
- Application

Run Order Wizard

Current method file : Obsidian.s2m
Current material : Obsidian

Run Order Wizard

Purpose
To create a "run order" file associated with this calibration. A run order is a file that automates the collection of spectra for samples.

How?
First use Bruker Instrument Tools to **copy the InstrumentDef.IDF** file from the instrument to the base folder of your EasyCal program. For example to "C:\Users\John\My Documents\Bruker\S1Cal\". If you have a Tracer 5^{i} you will also need to **copy \Bruker\System\ManualFilters.csv** to your base folder.

Then click on **Run Order Wizard** and ApplicationWizard will open Run Order Wizard for you.
Once open, choose the appropriate settings and click "OK".

The run order file has a ".csv" extension. It will be saved in the location indicated at the top of the Run Order Wizard program in a folder with the same name as the Calibration. For example "C:\Users\John\My Documents\Bruker\S1Cal\RunOrders\Alloys\Alloys.csv". Note that there are two additional files created in the same directory- S1-LineLibrary.xrd and S1-LineLibrary-A1.fll. Ignore these files.

Copy your run order file into a folder called "RunOrders" on a USB drive. You can do this directly by inserting the USB on the PC. Or by using BIT explorer with the USB inserted on the instrument and the instrument connected to the PC.

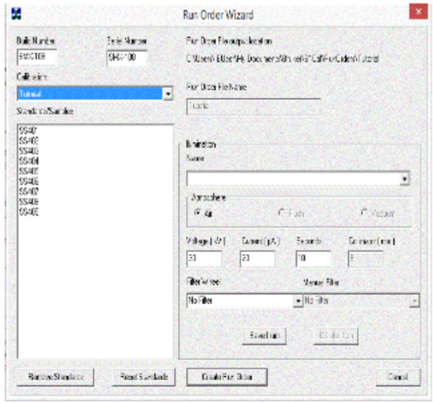
Insert the USB drive into the instrument.

Use the Run Order utility on the instrument to collect data from your samples. **(Ready-to-Test -> Utilities -> System Setup -> Run Order)**

The reference sample measurement files will be archived in a .7z type file in the SeqRun folder on the USB stick. The name of the file is identical to the Run Order.
When finished, remove the USB drive and put it back into the PC or transfer the files from SeqRun folder to the PC using BIT

Run **PDZ to SSD** to convevrt and copy the files to the required destination by the Wizard

Click *Run Order Wizard*



Run Order is the process Bruker uses internally to run calibration standards. You may use this to create an automatic data collector for your instrument

Regardless of whether you do or not, you do need to create a Run Order to tell EasyCal what to expect from your standards, and to define how your calibration will be applied

Obsidian.devm

For Help, press F1

Status

10:42 AM
5/1/18

ApplicationWizard - [Obsidian.devm *]

File Edit View Method Calibration Window Options Help

Obsidian
- Materials
  - Elements
  - Compounds
  - Standards
- Measurement
  - Run Order Wizard
  - PDZ to SSD
- Calibration
- Modules
- Application

Run Order Wizard

Current method file : Obsidian.s2m
Current material : Obsidian

Run Order Wizard

Purpose
To create a "run order" file associated with this calibration. A run order is a file that automates the collection of spectra for samples.

How?
First use Bruker Instrument Tools to **copy the InstrumentDef.IDF** file from the instrument to the base folder of your EasyCal program. For example to "C:\Users\John\My Documents\Bruker\S1Cal\". If you have a Tracer 5^{i} you will also need to **copy \Bruker\System\ManualFilters.csv** to your base folder.

Then click on **Run Order Wizard** and ApplicationWizard will open Run Order Wizard for you.
Once open, choose the appropriate settings and click "OK".

The run order file has a ".csv" extension. It will be saved in the location indicated at the top of the Run Order Wizard program in a folder with the same name as the Calibration. For example "C:\Users\John\My Documents\Bruke...\Alloys\Alloys.csv". Note that there are two additional files created in the same directory- S1-LineLibrary.xrd and S1-LineL...

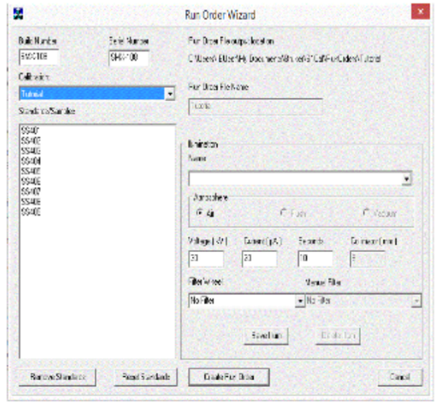
Copy your run order file into a folder called "RunOrders" on a USB drive. You can do t... BIT explorer with the USB inserted on the instrument and the instrument connected to...

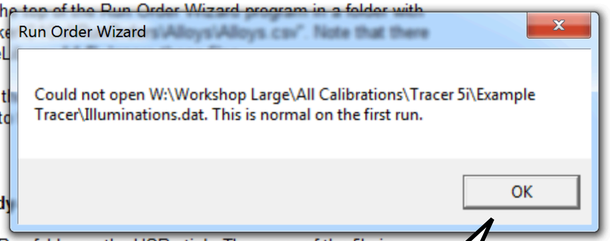
Insert the USB drive into the instrument.

Use the Run Order utility on the instrument to collect data from your samples. **(Ready...**

The reference sample measurement files will be archived in a .7z type file in the SeqRun folder on the USB stick. The name of the file is identical to the Run Order.
When finished, remove the USB drive and put it back into the PC or transfer the files from SeqRun folder to the PC using BIT

Run **PDZ to SSD** to convevrt and c...





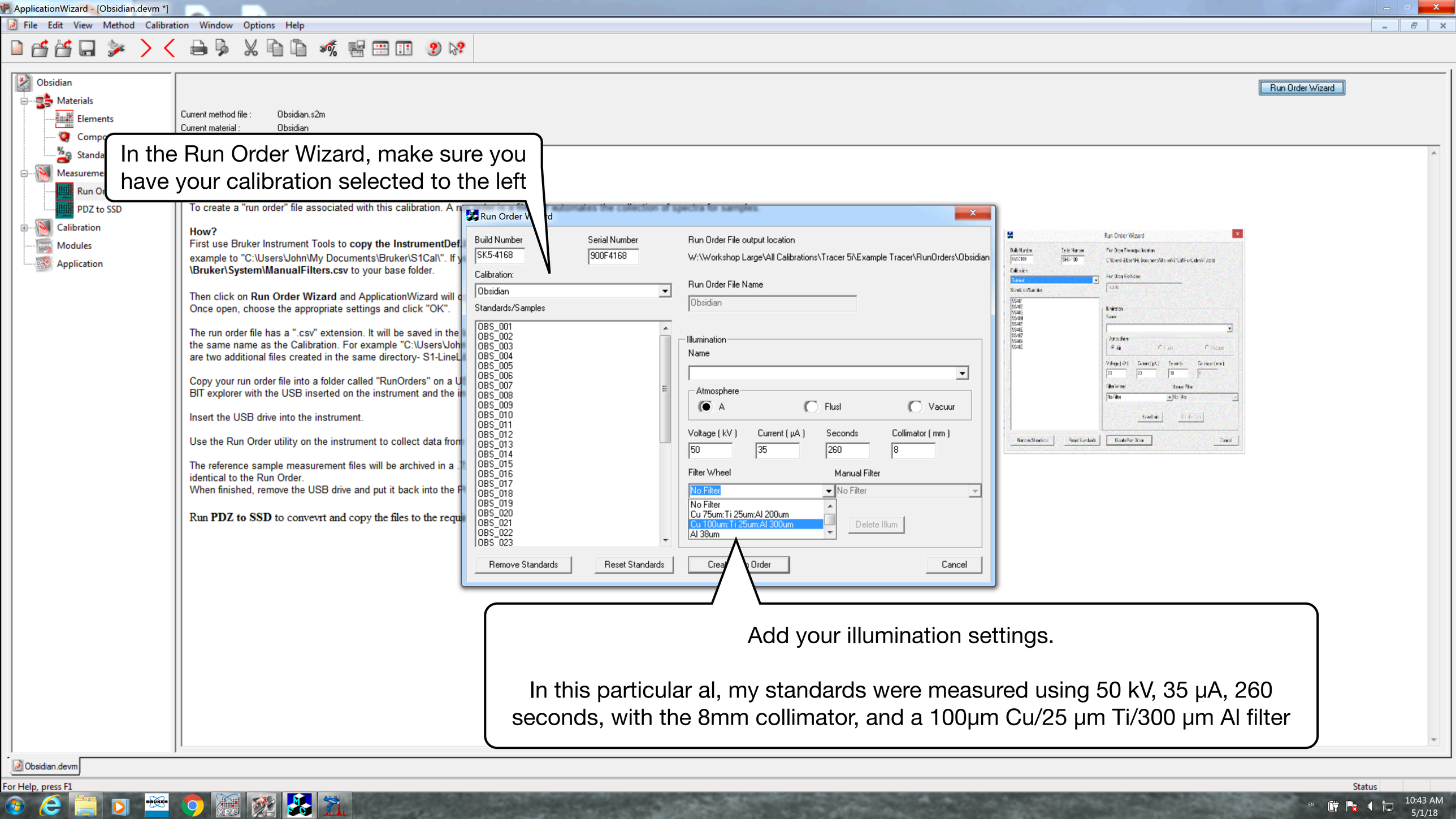
The first time you do a Run Order Wizard, it will look for Illuminations.dat - this is a file that stores your preferred voltage/ current/filter/atmosphere selections. It will create one the first time you use the software. Click *OK*

Obsidian.devm

For Help, press F1

Status

10:42 AM
5/1/18


ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Obsidian
Materials
Elements
Measureme
Run Or
PDZ to SSD
Calibration
Modules
Application
Run Order Wizard
Current method file : Obsidian.s2m
Current material : Obsidian
In the Run Order Wizard, make sure you have your calibration selected to the left
To create a "run order" file associated with this calibration. A r
How?
First use Bruker Instrument Tools to copy the InstrumentDef
example to "C:\Users\John\My Documents\Bruker\S1Cal\". If y
\Bruker\System\ManualFilters.csv to your base folder.
Then click on Run Order Wizard and ApplicationWizard will c
Once open, choose the appropriate settings and click "OK".
The run order file has a ".csv" extension. It will be saved in the
the same name as the Calibration. For example "C:\Users\Joh
are two additional files created in the same directory- S1-LineL
Copy your run order file into a folder called "RunOrders" on a U
BIT explorer with the USB inserted on the instrument and the it
Insert the USB drive into the instrument.
Use the Run Order utility on the instrument to collect data fron
The reference sample measurement files will be archived in a .
identical to the Run Order.
When finished, remove the USB drive and put it back into the F
Run PDZ to SSD to convevrt and copy the files to the requ
Run Order W d
Build Number
SK5-4168
Serial Number
900F4168
Run Order File output location
W:\Workshop Large\All Calibrations\Tracer 5i\Example Tracer\RunOrders\Obsidian
Calibration:
Obsidian
Run Order File Name
Obsidian
Standards/Samples
OBS_001
OBS_002
OBS_003
OBS_004
OBS_005
OBS_006
OBS_007
OBS_008
OBS_009
OBS_010
OBS_011
OBS_012
OBS_013
OBS_014
OBS_015
OBS_016
OBS_017
OBS_018
OBS_019
OBS_020
OBS_021
OBS_022
OBS_023
Illumination
Name
Atmosphere
A
Flusl
Vacuur
Voltage (kV)
50
Current (µA)
35
Seconds
260
Collimator (mm)
8
Filter Wheel
No Filter
Manual Filter
No Filter
No Filter
Cu 75um:Ti 25um:Al 200um
Cu 100um:Ti 25um:Al 300um
Al 38um
Delete Illum
Remove Standards
Reset Standards
Cancel
Add your illumination settings.
In this particular al, my standards were measured using 50 kV, 35 µA, 260 seconds, with the 8mm collimator, and a 100µm Cu/25 µm Ti/300 µm Al filter
Obsidian.devm
For Help, press F1
Status
10:43 AM
5/1/18

ApplicationWizard - [Obsidian.devm *]

File Edit View Method Calibration Window Options Help

Obsidian
- Materials
  - Elements
  - Compounds
  - Standards
- Measurement
  - Run Order Wizard
  - PDZ to SSD
- Calibration
- Modules
- Application

Run Order Wizard

Current method file : Obsidian.s2m
Current material : Obsidian

Run Order Wizard

Purpose
To create a "run or

How?
First use Bruker In
example to "C:\Us
\Bruker\System\M

Then click on **Run Order Wizard** and ApplicationWizard will
Once open, choose the appropriate settings and click "OK".

The run order file has a ".csv" extension. It will be saved in the
the same name as the Calibration. For example "C:\Users\Joh
are two additional files created in the same directory- S1-LineL

Copy your run order file into a folder called "RunOrders" on a U
BIT explorer with the USB inserted on the instrument and the i

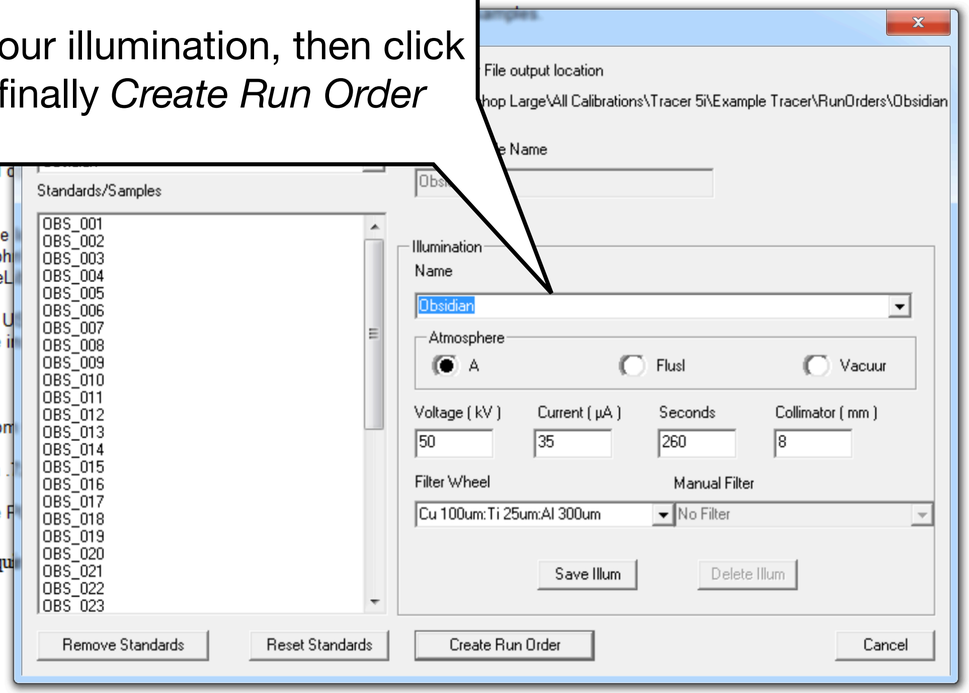
Insert the USB drive into the instrument.

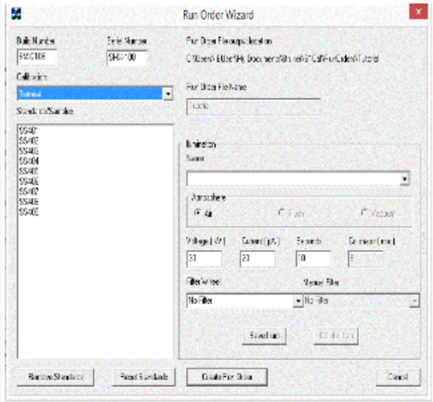
Use the Run Order utility on the instrument to collect data fro

The reference sample measurement files will be archived in a .
identical to the Run Order.
When finished, remove the USB drive and put it back into the

Run PDZ to SSD to convevrt and copy the files to the requ

Give a name to your illumination, then click *Save Ilum* and finally *Create Run Order*





Obsidian.devm

For Help, press F1

Status

10:43 AM
5/1/18

ApplicationWizard - [Obsidian.devm *]

File Edit View Method Calibration Window Options Help

Click on the red forward > button and move to the next step

Obsidian
- Materials
  - Elements
  - Compounds
  - Standards
- Measurement
  - Run Order Wizard
  - PDZ to SSD
- Calibration
- Modules
- Application

Run Order Wizard

Current method file : Obsidi
Current material : Obsidian

Run Order Wizard

Purpose
To create a "run order" file associated

How?
First use Bruker Instrument Tools to c
example to "C:\Users\John\My Docur
\Bruker\System\ManualFilters.csv t

Then click on **Run Order Wizard** and
Once open, choose the appropriate s

The run order file has a ".csv" extensi
the same name as the Calibration. Fo
are two additional files created in the

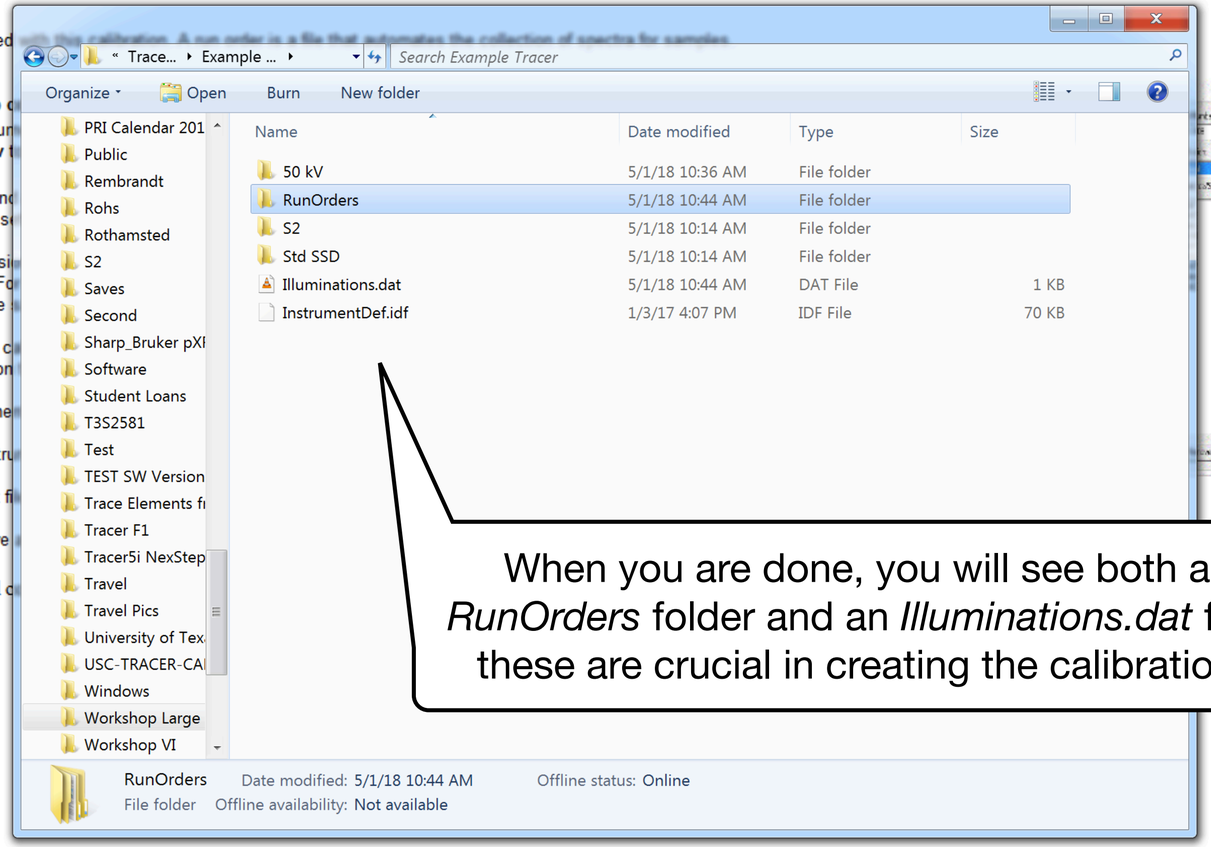
Copy your run order file into a folder c
BIT explorer with the USB inserted on

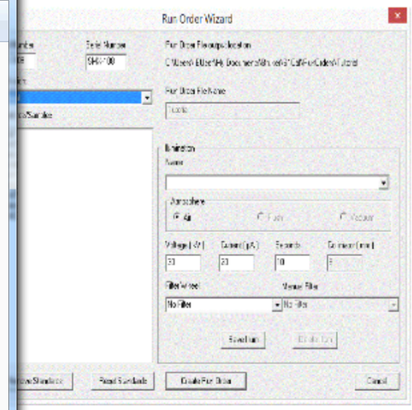
Insert the USB drive into the instrume

Use the Run Order utility on the instru

The reference sample measurement fi
identical to the Run Order.
When finished, remove the USB drive

Run **PDZ to SSD** to convevrt and c





When you are done, you will see both a *RunOrders* folder and an *Illuminations.dat* file, these are crucial in creating the calibration

Obsidian.devm

For Help, press F1

Status

EN 10:44 AM 5/1/18

ApplicationWizard - [Obsidian.devm *]

File Edit View Method Calibration Window Options Help

Obsidian
- Materials
  - Elements
  - Compounds
  - Standards
- Measurement
  - Run Order Wizard
  - PDZ to SSD
- Calibration
- Modules
- Application

Current method file : Obsidian.s2m
Current material : Obsidian

PDZ to SSD

Click on *PDZ to SSD*

PDZ to SSD

Purpose

To convert the data files, acquired as a 7z file with the Run Order Wizard, from .pdz to .ssd format. EasyCal requires the ssd format.

How?

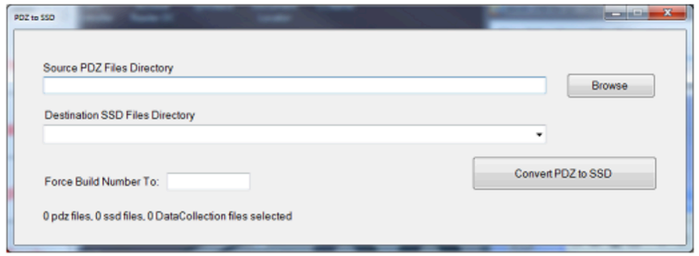
Use the **Browse** button to navigate to the location of the 7z data file.

Select the destination folder from the **drop down menu**. The appropiate folder should end with the name of the calibration

Click **Convert PDZ to SSD** to complete the conversion (use (X) to exit).

Special feature:

If data comes from other instruments you can overwrite the **Build Number**. (This is not recommended, all data should be taken with the instrument for which the calibration is intended.)



On *PDZ to SSD*, we convert any PDZ files to SSD files. This process also automatically sorts your data to be useable by the app

Obsidian.devm

For Help, press F1

Status

10:44 AM
5/1/18

PDZ to SSD

Source PDZ Files Directory

Browse

Destination SSD Files Directory

Force Build Number To:

Convert PDZ to SSD

0 pdz files, 0 ssd files, 0 DataCollection files selected

PDZ to SSD

Calibration
Modules
Application

al requires the ssd format.

How?

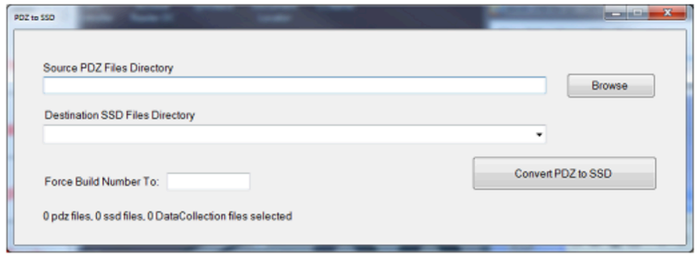
Use the **Browse** button to navigate to the locati of the 7z data file.

Select the destination folder from the **drop down enu**. The appropiate folder should end with the name of the calibration

Click **Convert PDZ to SSD** to complete the conve n (use (X) to exit).

Special feature:

If data comes from other instruments you can over e **Build Number**. (This is not recommended, all data should be taken with the instrument for which the calibration is intended.)



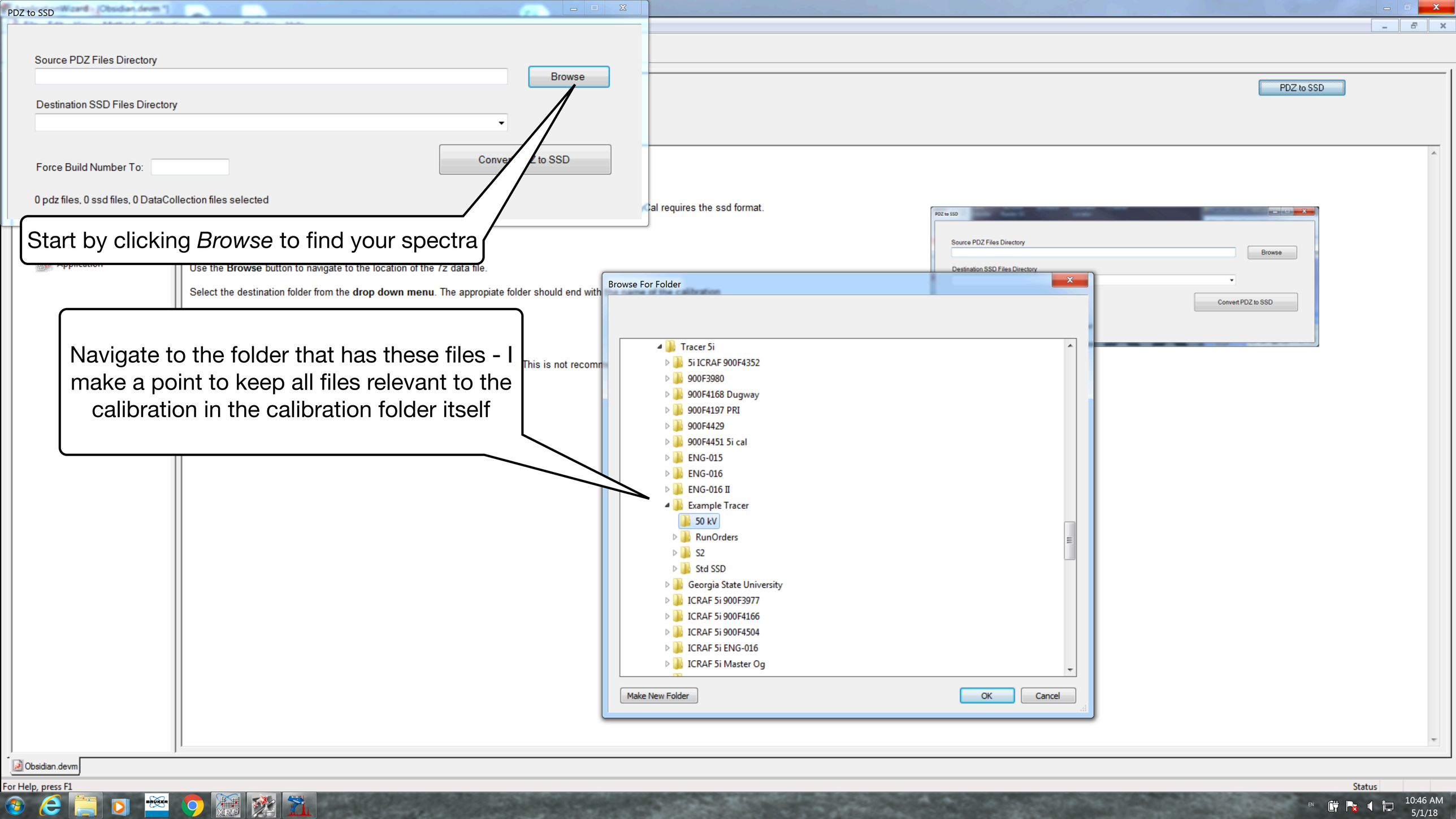
This opens a window to convert and organize files to be used by EasyCal

Obsidian.devm

For Help, press F1

Status

10:44 AM
5/1/18


PDZ to SSD
Source PDZ Files Directory
Browse
Destination SSD Files Directory
Force Build Number To:
Convert PDZ to SSD
0 pdz files, 0 ssd files, 0 DataCollection files selected
Start by clicking *Browse* to find your spectra
Navigate to the folder that has these files - I make a point to keep all files relevant to the calibration in the calibration folder itself
Browse For Folder
Tracer 5i
5i ICRAF 900F4352
900F3980
900F4168 Dugway
900F4197 PRI
900F4429
900F4451 5i cal
ENG-015
ENG-016
ENG-016 II
Example Tracer
50 kV
RunOrders
S2
Std SSD
Georgia State University
ICRAF 5i 900F3977
ICRAF 5i 900F4166
ICRAF 5i 900F4504
ICRAF 5i ENG-016
ICRAF 5i Master Og
Make New Folder
OK
Cancel
Use the Browse button to navigate to the location of the .tz data file.
Select the destination folder from the drop down menu. The appropiate folder should end with
Obsidian.devm
For Help, press F1
Status
10:46 AM
5/1/18

PDZ to SSD

Source PDZ Files Directory

W:\Workshop Large\All Calibrations\Tracer 5i\Example Tracer\50 kV

Browse

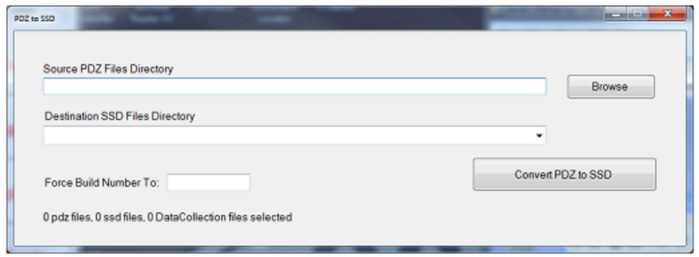
Destination SSD Files Directory

Force Build Number To:

Convert PDZ to SSD

40 pdz files, 0 ssd files, 0 DataCollection files selected

You will see that folder's path in the window. The number of PDZ files in that directory will be in the lower left



You don't have to use folders - the *Source PDZ Files Directory* can also open up compressed .7z folders produced automatically by the instrument.

PDZ to SSD

Source PDZ Files Directory

W:\Workshop Large\All Calibrations\Tracer 5i\Example Tracer\50 kV

Browse

Destination SSD Files Directory

W:\Workshop Large\All Calibrations\Tracer 5i\Example Tracer\Std SSD\Libraries\Materials\Obsidian\Sol

Force Build Number To:

Convert PDZ to SSD

40 pdz files, 0 ssd files, 0 DataCollection files selected

PDZ to SSD

Calibration

Modules

Application

al requires the ssd format.

How?

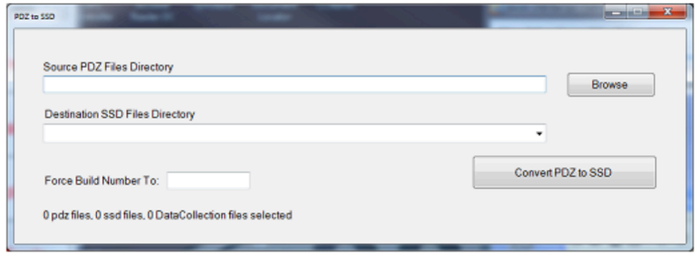
Use the **Browse** button to navigate to the location of the 7z data file.

Select the destination folder from the **drop down menu**. The appropiate folder should the name of the calibration

Click **Convert PDZ to SSD** to complete the conversion (use (X) to exit).

Speci

If data
instru



Next, click the down arrow and choose the folder for your calibration. There is only one now, but each new calibration will add one to this list

Obsidian.devm

For Help, press F1

Status

10:46 AM
5/1/18

PDZ to SSD

Source PDZ Files Directory

W:\Workshop Large\All Calibrations\Tracer 5i\Example Tracer\50 kV

Browse

Destination SSD Files Directory

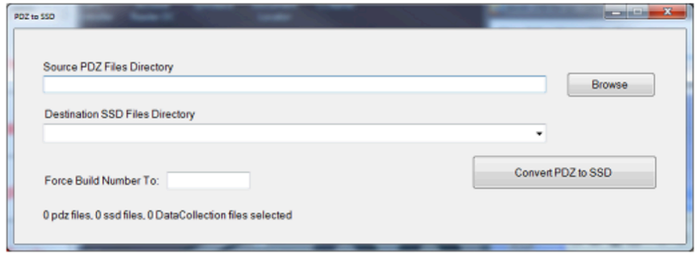
orkshop Large\All Calibrations\Tracer 5i\Example Tracer\Std SSD\Libraries\Materials\Obsidian\Solids

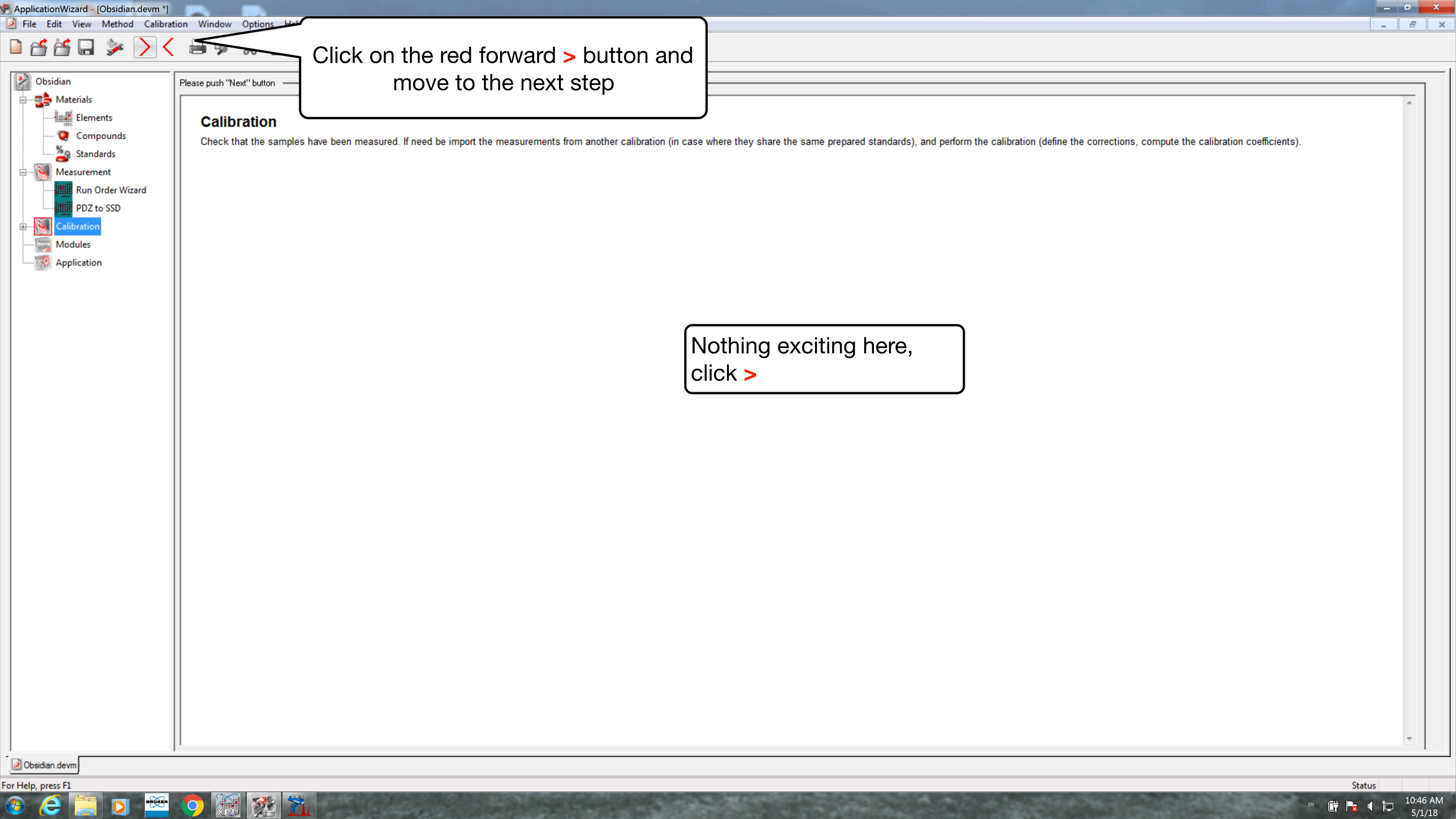
Force Build Number To:

Convert PDZ to SSD

40 pdz files, 0 ssd files, 0 DataCollection files selected

When you have selected both a source and destination folder, you can then click *Convert PDZ to SSD*




ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options Help
Click on the red forward > button and move to the next step
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Modules
Application
Please push "Next" button
Calibration
Check that the samples have been measured. If need be import the measurements from another calibration (in case where they share the same prepared standards), and perform the calibration (define the corrections, compute the calibration coefficients).
Nothing exciting here, click >
Obsidian.devm
For Help, press F1
Status
10:46 AM
5/1/18

ApplicationWizard - [Obsidian.devm *]

File Edit View Method Calibration Window Options Help

Obsidian
- Materials
  - Elements
  - Compounds
  - Standards
- Measurement
  - Run Order Wizard
  - PDZ to SSD
- Calibration
  - Manage Standards
  - Compute
- Modules
- Application

Data files path: W:\Workshop Large\All Calibrations\Tracer 5i\Example Tracer\Std SSD\Libraries\Materials\Obsidian\Solids\

Disable missing stds. | Disable invalid stds. | Import more stds.

Samples: 40 Selected: 40

Prepared standards	Imported	Material	Preparation	File
OBS_001_Solids		Obsidian	Solids	Exist
OBS_002_Solids		Obsidian	Solids	Exist
OBS_003_Solids		Obsidian	Solids	Exist
OBS_004_Solids		Obsidian	Solids	Exist
OBS_005_Solids		Obsidian	Solids	Exist
OBS_006_Solids		Obsidian	Solids	Exist
OBS_007_Solids		Obsidian	Solids	Exist
OBS_008_Solids		Obsidian	Solids	Exist
OBS_009_Solids		Obsidian	Solids	Exist
OBS_010_Solids		Obsidian	Solids	Exist
OBS_011_Solids		Obsidian	Solids	Exist
OBS_012_Solids		Obsidian	Solids	Exist
OBS_013_Solids		Obsidian	Solids	Exist
OBS_014_Solids		Obsidian	Solids	Exist
OBS_015_Solids		Obsidian	Solids	Exist
OBS_016_Solids		Obsidian	Solids	Exist
OBS_017_Solids		Obsidian	Solids	Exist
OBS_018_Solids		Obsidian	Solids	Exist
OBS_019_Solids		Obsidian	Solids	Exist
OBS_020_Solids		Obsidian	Solids	Exist
OBS_021_Solids		Obsidian	Solids	Exist
OBS_022_Solids		Obsidian	Solids	Exist
OBS_023_Solids		Obsidian	Solids	Exist
OBS_024_Solids		Obsidian	Solids	Exist
OBS_025_Solids		Obsidian	Solids	Exist
OBS_026_Solids		Obsidian	Solids	Exist
OBS_027_Solids		Obsidian	Solids	Exist
OBS_028_Solids		Obsidian	Solids	Exist
OBS_029_Solids		Obsidian	Solids	Exist
OBS_030_Solids		Obsidian	Solids	Exist
OBS_031_Solids		Obsidian	Solids	Exist
OBS_032_Solids		Obsidian	Solids	Exist
OBS_033_Solids		Obsidian	Solids	Exist
OBS_034_Solids		Obsidian	Solids	Exist
OBS_035_Solids		Obsidian	Solids	Exist
OBS_036_Solids		Obsidian	Solids	Exist
OBS_037_Solids		Obsidian	Solids	Exist
OBS_038_Solids		Obsidian	Solids	Exist
OBS_039_Solids		Obsidian	Solids	Exist
OBS_040_Solids		Obsidian	Solids	Exist

In *Manage Standards*, we can see our standards. If we have both the quantitative values and the spectra matched, it will say *Exist*

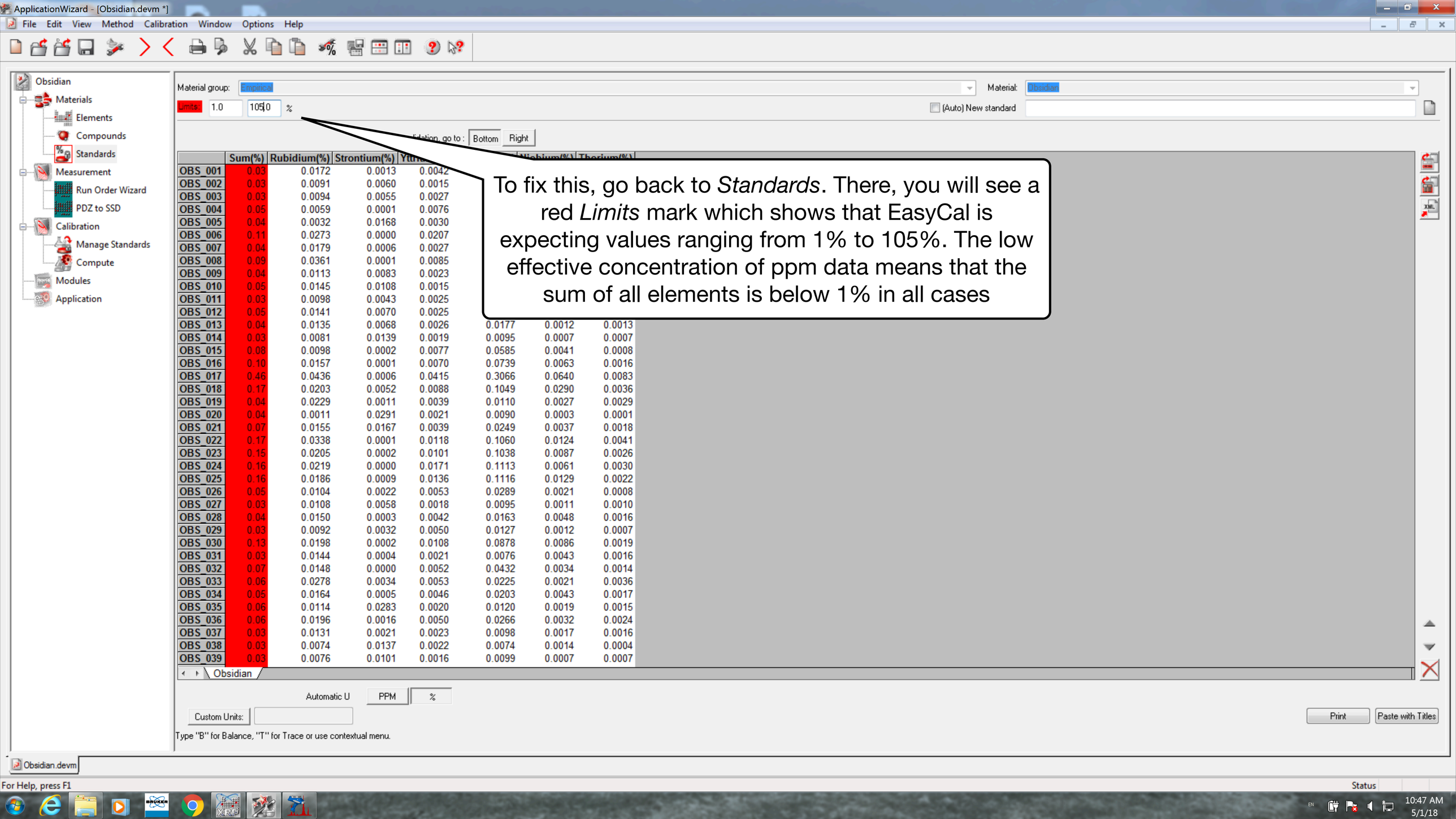
But a problem - all of these have red check marks. This is because the standards are in ppm units, so EasyCal doesn't think you have enough to work with

Obsidian.devm

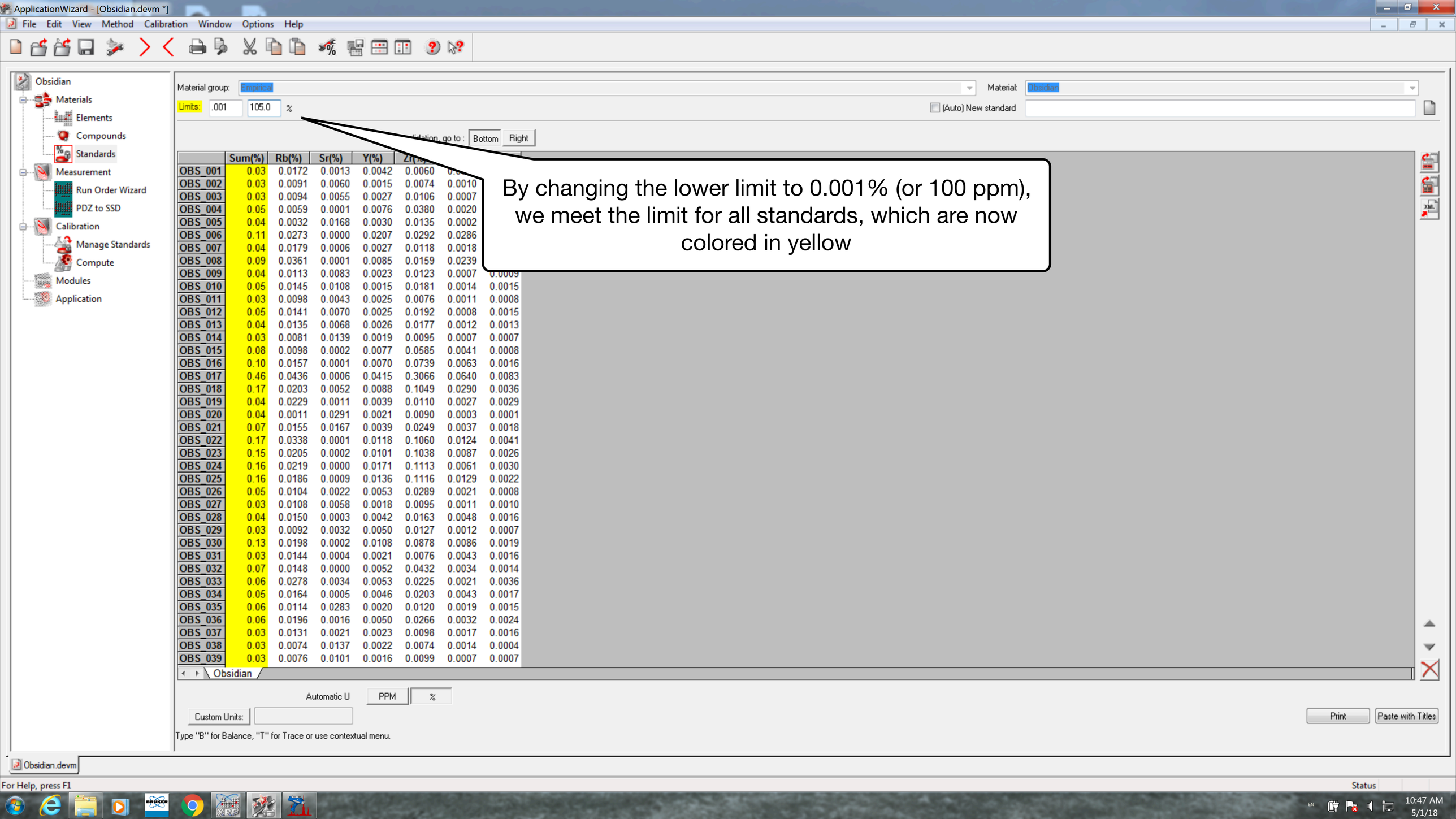
For Help, press F1

Status

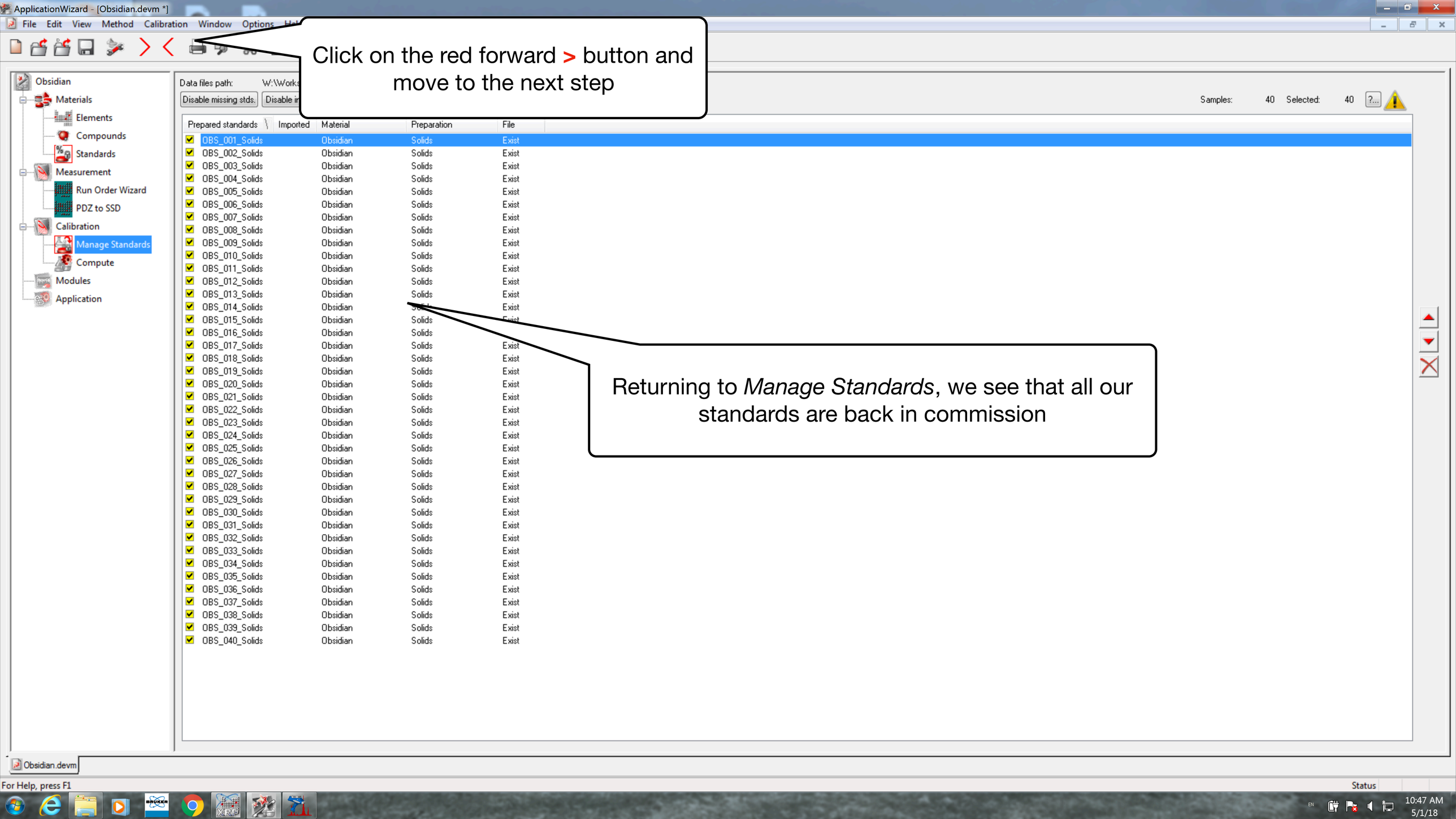
10:46 AM
5/1/18



	Sum(%)	Rubidium(%)	Strontium(%)	Yttrium(%)	Niobium(%)	Thorium(%)
OBS_001	0.03	0.0172	0.0013	0.0042		
OBS_002	0.03	0.0091	0.0060	0.0015		
OBS_003	0.03	0.0094	0.0055	0.0027		
OBS_004	0.05	0.0059	0.0001	0.0076		
OBS_005	0.04	0.0032	0.0168	0.0030		
OBS_006	0.11	0.0273	0.0000	0.0207		
OBS_007	0.04	0.0179	0.0006	0.0027		
OBS_008	0.09	0.0361	0.0001	0.0085		
OBS_009	0.04	0.0113	0.0083	0.0023		
OBS_010	0.05	0.0145	0.0108	0.0015		
OBS_011	0.03	0.0098	0.0043	0.0025		
OBS_012	0.05	0.0141	0.0070	0.0025		
OBS_013	0.04	0.0135	0.0068	0.0026	0.0177	0.0012	0.0013
OBS_014	0.03	0.0081	0.0139	0.0019	0.0095	0.0007	0.0007
OBS_015	0.08	0.0098	0.0002	0.0077	0.0585	0.0041	0.0008
OBS_016	0.10	0.0157	0.0001	0.0070	0.0739	0.0063	0.0016
OBS_017	0.46	0.0436	0.0006	0.0415	0.3066	0.0640	0.0083
OBS_018	0.17	0.0203	0.0052	0.0088	0.1049	0.0290	0.0036
OBS_019	0.04	0.0229	0.0011	0.0039	0.0110	0.0027	0.0029
OBS_020	0.04	0.0011	0.0291	0.0021	0.0090	0.0003	0.0001
OBS_021	0.07	0.0155	0.0167	0.0039	0.0249	0.0037	0.0018
OBS_022	0.17	0.0338	0.0001	0.0118	0.1060	0.0124	0.0041
OBS_023	0.15	0.0205	0.0002	0.0101	0.1038	0.0087	0.0026
OBS_024	0.16	0.0219	0.0000	0.0171	0.1113	0.0061	0.0030
OBS_025	0.16	0.0186	0.0009	0.0136	0.1116	0.0129	0.0022
OBS_026	0.05	0.0104	0.0022	0.0053	0.0289	0.0021	0.0008
OBS_027	0.03	0.0108	0.0058	0.0018	0.0095	0.0011	0.0010
OBS_028	0.04	0.0150	0.0003	0.0042	0.0163	0.0048	0.0016
OBS_029	0.03	0.0092	0.0032	0.0050	0.0127	0.0012	0.0007
OBS_030	0.13	0.0198	0.0002	0.0108	0.0878	0.0086	0.0019
OBS_031	0.03	0.0144	0.0004	0.0021	0.0076	0.0043	0.0016
OBS_032	0.07	0.0148	0.0000	0.0052	0.0432	0.0034	0.0014
OBS_033	0.06	0.0278	0.0034	0.0053	0.0225	0.0021	0.0036
OBS_034	0.05	0.0164	0.0005	0.0046	0.0203	0.0043	0.0017
OBS_035	0.06	0.0114	0.0283	0.0020	0.0120	0.0019	0.0015
OBS_036	0.06	0.0196	0.0016	0.0050	0.0266	0.0032	0.0024
OBS_037	0.03	0.0131	0.0021	0.0023	0.0098	0.0017	0.0016
OBS_038	0.03	0.0074	0.0137	0.0022	0.0074	0.0014	0.0004
OBS_039	0.03	0.0076	0.0101	0.0016	0.0099	0.0007	0.0007



	Sum(%)	Rb(%)	Sr(%)	Y(%)	Zr(%)	
OBS_001	0.03	0.0172	0.0013	0.0042	0.0060	
OBS_002	0.03	0.0091	0.0060	0.0015	0.0074	0.0010
OBS_003	0.03	0.0094	0.0055	0.0027	0.0106	0.0007
OBS_004	0.05	0.0059	0.0001	0.0076	0.0380	0.0020
OBS_005	0.04	0.0032	0.0168	0.0030	0.0135	0.0002
OBS_006	0.11	0.0273	0.0000	0.0207	0.0292	0.0286
OBS_007	0.04	0.0179	0.0006	0.0027	0.0118	0.0018
OBS_008	0.09	0.0361	0.0001	0.0085	0.0159	0.0239
OBS_009	0.04	0.0113	0.0083	0.0023	0.0123	0.0007
OBS_010	0.05	0.0145	0.0108	0.0015	0.0181	0.0014
OBS_011	0.03	0.0098	0.0043	0.0025	0.0076	0.0011
OBS_012	0.05	0.0141	0.0070	0.0025	0.0192	0.0008
OBS_013	0.04	0.0135	0.0068	0.0026	0.0177	0.0012
OBS_014	0.03	0.0081	0.0139	0.0019	0.0095	0.0007
OBS_015	0.08	0.0098	0.0002	0.0077	0.0585	0.0041
OBS_016	0.10	0.0157	0.0001	0.0070	0.0739	0.0063
OBS_017	0.46	0.0436	0.0006	0.0415	0.3066	0.0640
OBS_018	0.17	0.0203	0.0052	0.0088	0.1049	0.0290
OBS_019	0.04	0.0229	0.0011	0.0039	0.0110	0.0027
OBS_020	0.04	0.0011	0.0291	0.0021	0.0090	0.0003
OBS_021	0.07	0.0155	0.0167	0.0039	0.0249	0.0037
OBS_022	0.17	0.0338	0.0001	0.0118	0.1060	0.0124
OBS_023	0.15	0.0205	0.0002	0.0101	0.1038	0.0087
OBS_024	0.16	0.0219	0.0000	0.0171	0.1113	0.0061
OBS_025	0.16	0.0186	0.0009	0.0136	0.1116	0.0129
OBS_026	0.05	0.0104	0.0022	0.0053	0.0289	0.0021
OBS_027	0.03	0.0108	0.0058	0.0018	0.0095	0.0011
OBS_028	0.04	0.0150	0.0003	0.0042	0.0163	0.0048
OBS_029	0.03	0.0092	0.0032	0.0050	0.0127	0.0012
OBS_030	0.13	0.0198	0.0002	0.0108	0.0878	0.0086
OBS_031	0.03	0.0144	0.0004	0.0021	0.0076	0.0043
OBS_032	0.07	0.0148	0.0000	0.0052	0.0432	0.0034
OBS_033	0.06	0.0278	0.0034	0.0053	0.0225	0.0021
OBS_034	0.05	0.0164	0.0005	0.0046	0.0203	0.0043
OBS_035	0.06	0.0114	0.0283	0.0020	0.0120	0.0019
OBS_036	0.06	0.0196	0.0016	0.0050	0.0266	0.0032
OBS_037	0.03	0.0131	0.0021	0.0023	0.0098	0.0017
OBS_038	0.03	0.0074	0.0137	0.0022	0.0074	0.0014
OBS_039	0.03	0.0076	0.0101	0.0016	0.0099	0.0007


ApplicationWizard - [Obsidian.devm *]
File Edit View Method Calibration Window Options
Click on the red forward > button and move to the next step
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Modules
Application
Data files path:
Disable missing stds.
Samples: 40 Selected: 40
Prepared standards | Imported | Material | Preparation | File
OBS_001_Solids Obsidian Solids Exist
OBS_002_Solids Obsidian Solids Exist
OBS_003_Solids Obsidian Solids Exist
OBS_004_Solids Obsidian Solids Exist
OBS_005_Solids Obsidian Solids Exist
OBS_006_Solids Obsidian Solids Exist
OBS_007_Solids Obsidian Solids Exist
OBS_008_Solids Obsidian Solids Exist
OBS_009_Solids Obsidian Solids Exist
OBS_010_Solids Obsidian Solids Exist
OBS_011_Solids Obsidian Solids Exist
OBS_012_Solids Obsidian Solids Exist
OBS_013_Solids Obsidian Solids Exist
OBS_014_Solids Obsidian Exist
OBS_015_Solids Obsidian Solids
OBS_016_Solids Obsidian Solids
OBS_017_Solids Obsidian Solids Exist
OBS_018_Solids Obsidian Solids Exist
OBS_019_Solids Obsidian Solids Exist
OBS_020_Solids Obsidian Solids Exist
OBS_021_Solids Obsidian Solids Exist
OBS_022_Solids Obsidian Solids Exist
OBS_023_Solids Obsidian Solids Exist
OBS_024_Solids Obsidian Solids Exist
OBS_025_Solids Obsidian Solids Exist
OBS_026_Solids Obsidian Solids Exist
OBS_027_Solids Obsidian Solids Exist
OBS_028_Solids Obsidian Solids Exist
OBS_029_Solids Obsidian Solids Exist
OBS_030_Solids Obsidian Solids Exist
OBS_031_Solids Obsidian Solids Exist
OBS_032_Solids Obsidian Solids Exist
OBS_033_Solids Obsidian Solids Exist
OBS_034_Solids Obsidian Solids Exist
OBS_035_Solids Obsidian Solids Exist
OBS_036_Solids Obsidian Solids Exist
OBS_037_Solids Obsidian Solids Exist
OBS_038_Solids Obsidian Solids Exist
OBS_039_Solids Obsidian Solids Exist
OBS_040_Solids Obsidian Solids Exist
Returning to Manage Standards, we see that all our standards are back in commission
Obsidian.devm
For Help, press F1
Status
10:47 AM
5/1/18

We are now ready to begin creating the calibration. There are a number of options you can consider

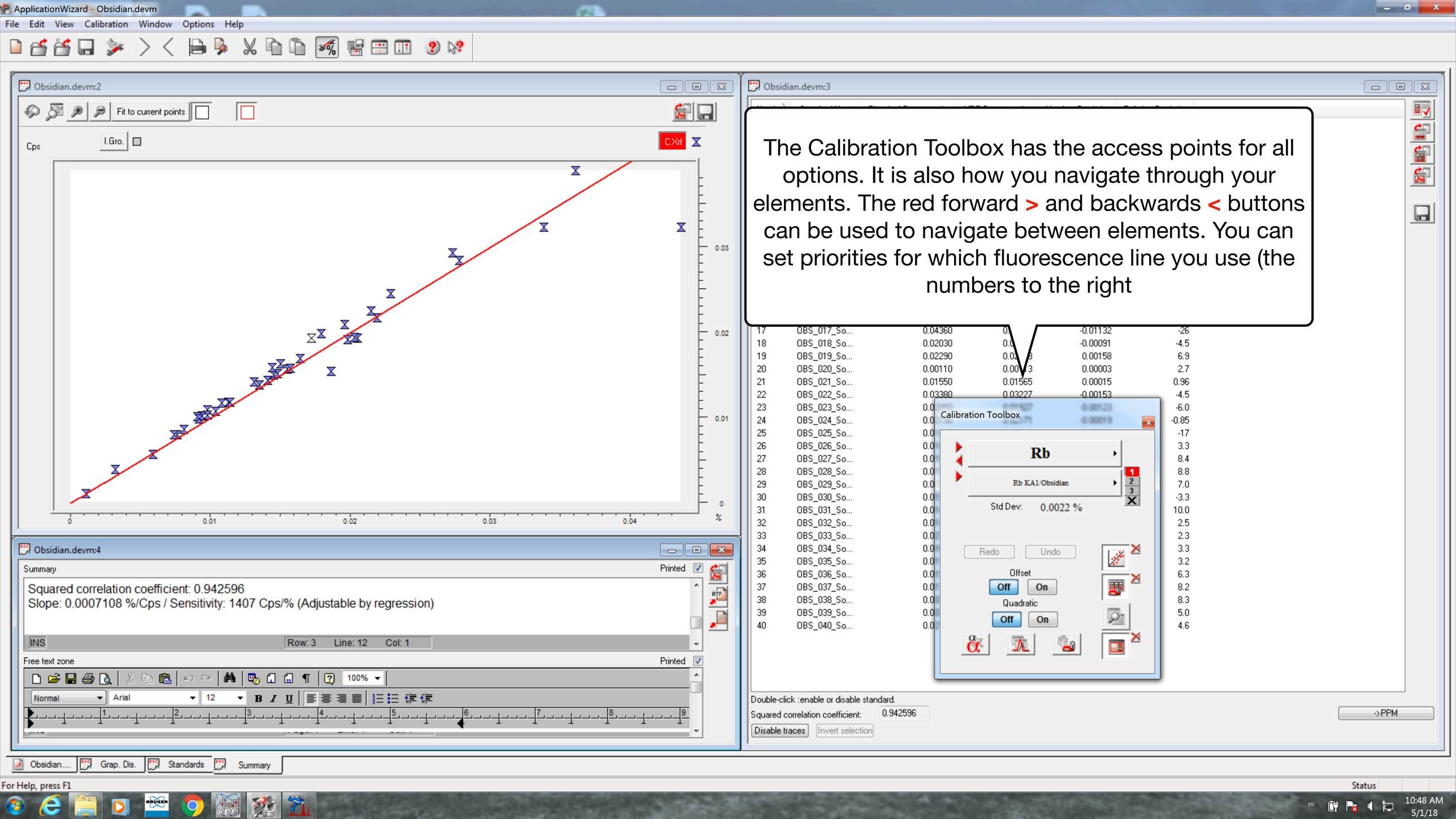
- **Internal Standard** (normalization): You can normalize by time or Compton (18.4 - 19.4 keV)

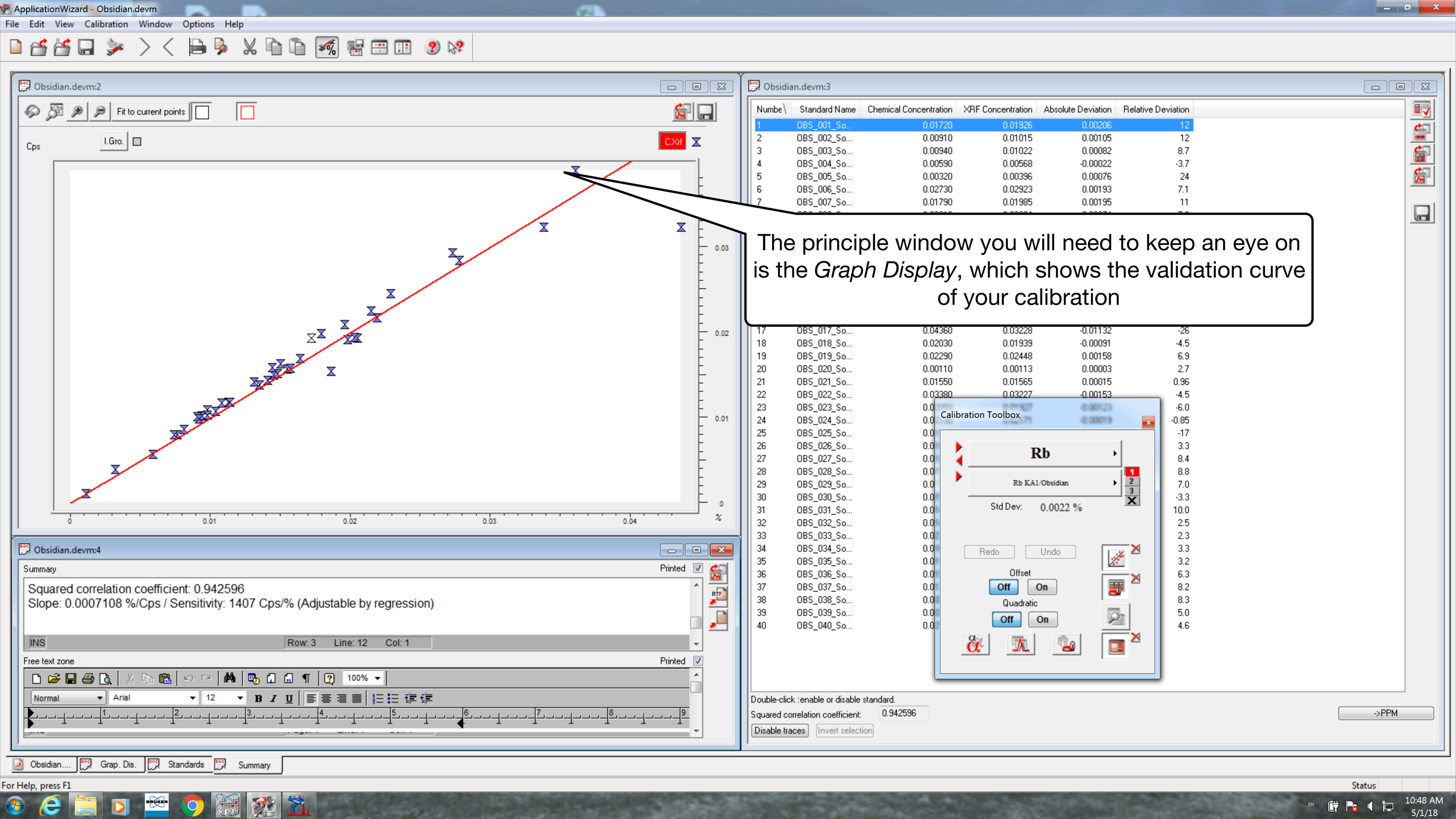
- **Line Overlap**: You can subtract an element which has a fluorescence line overlap with another.

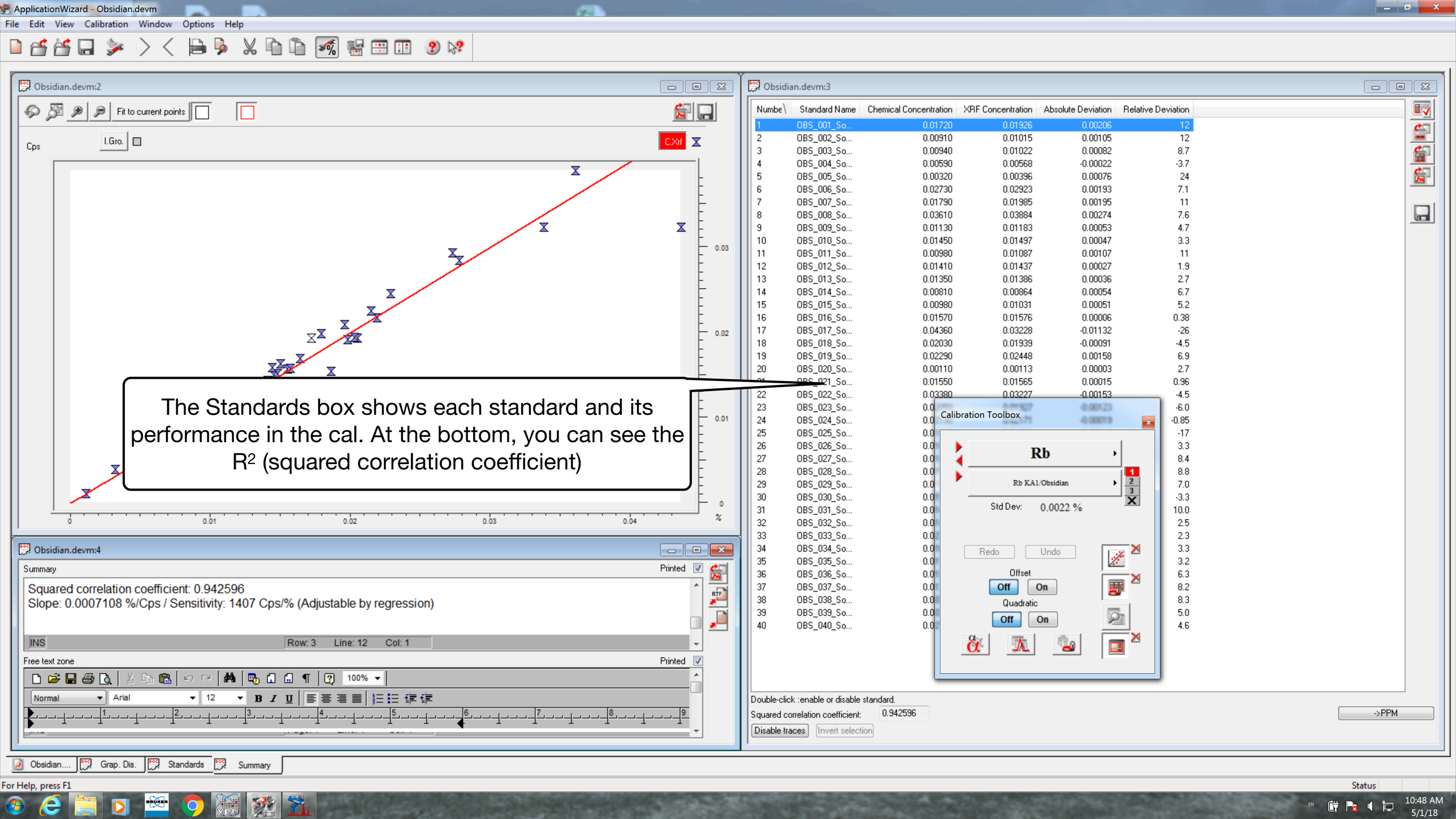
- **Alphas** (slope corrections): You can use an element as a predictor in the event it influences the element's fluorescence

- **Offset**: This ground the calibration, and in most other calibration software is the default setting

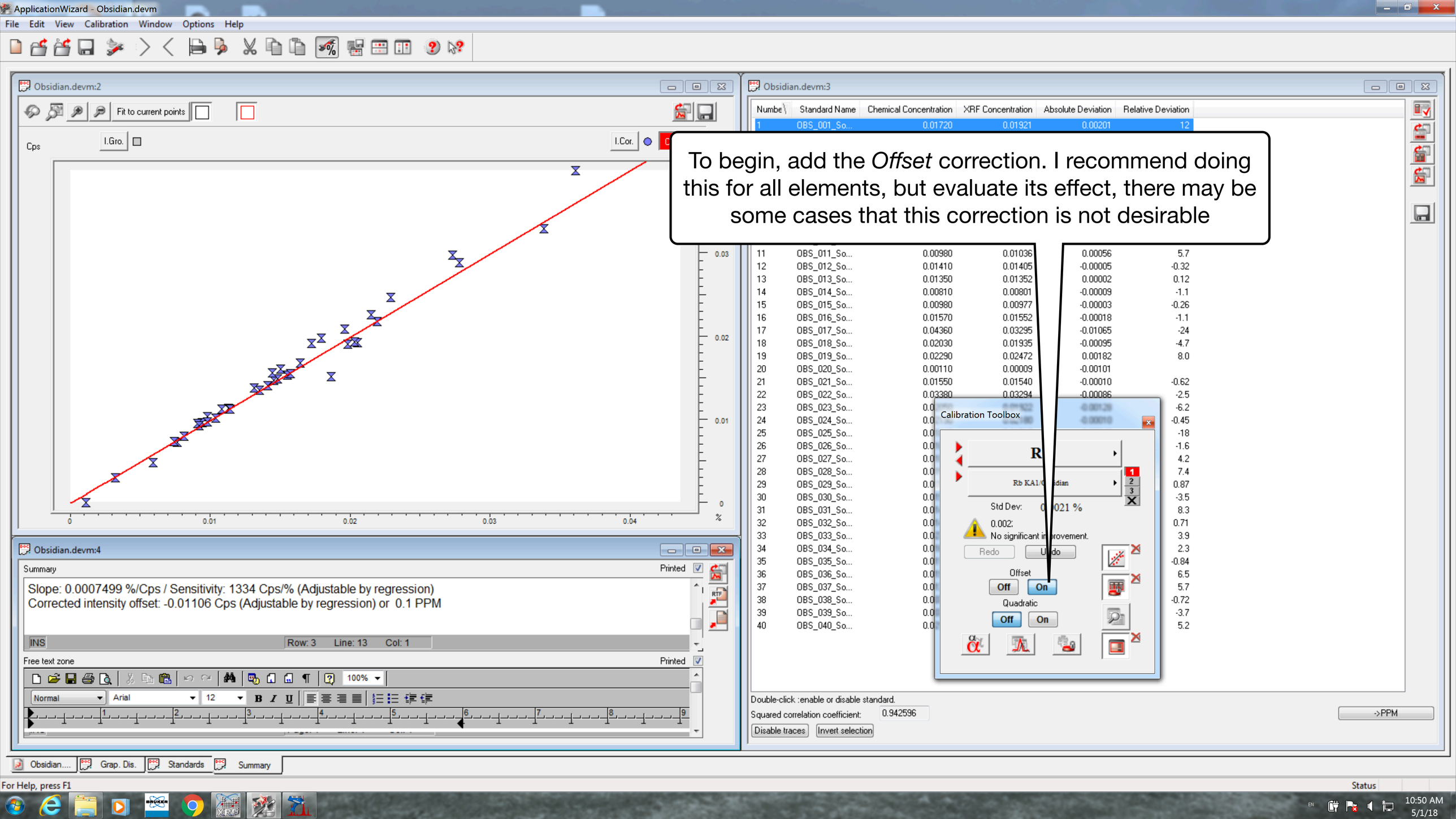
- **Quadratic**: This uses a second-order polynomial, rather than linear, regression

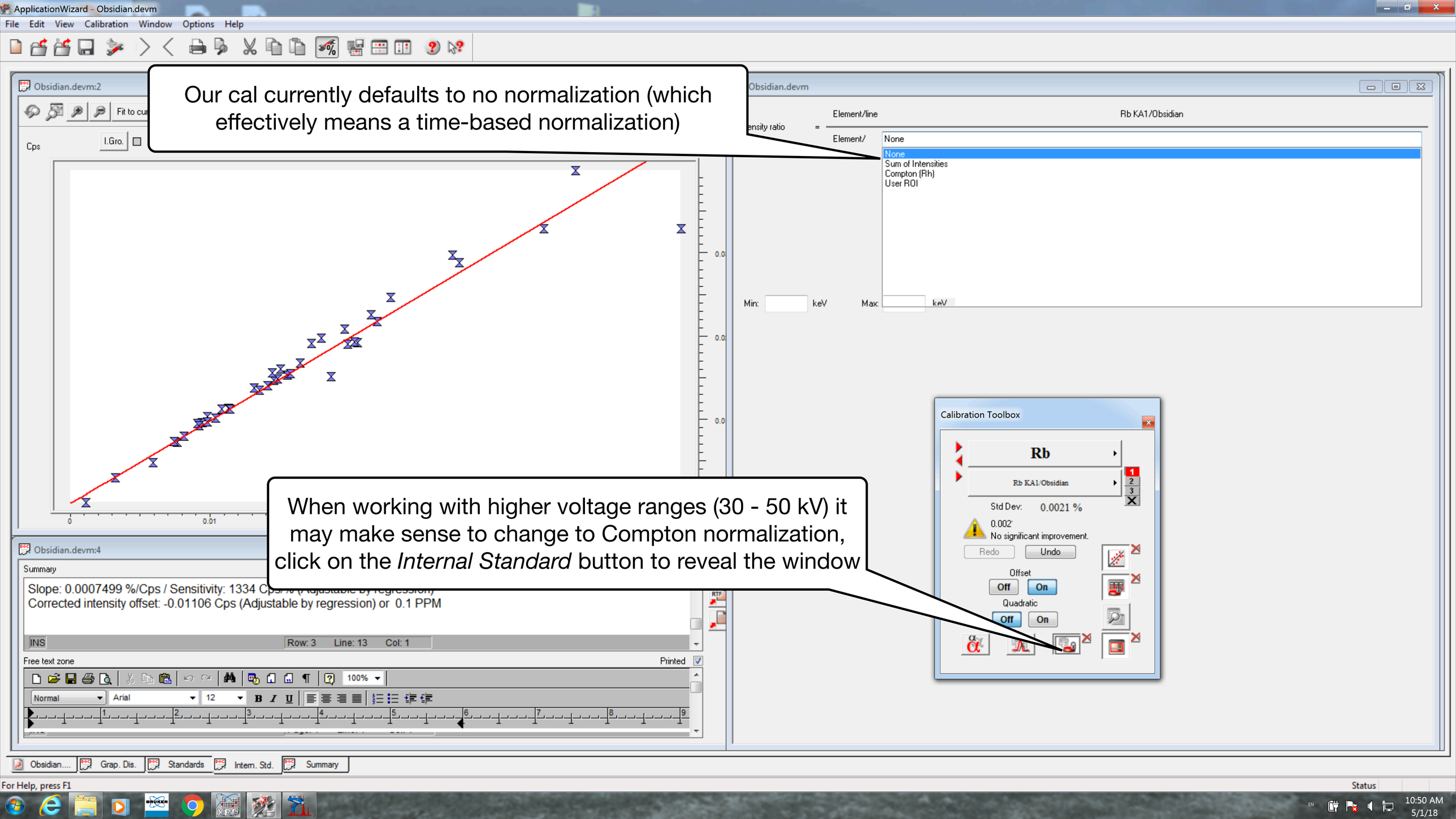

ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
CXrf
0.03
0.02
0.01
0
0.01
0.02
0.03
0.04
%
Obsidian.devm:4
Summary
Printed
Squared correlation coefficient: 0.942596
Slope: 0.0007108 %/Cps / Sensitivity: 1407 Cps/% (Adjustable by regression)
INS
Row: 3 Line: 12 Col: 1
Free text zone
Printed
100%
Normal
Arial
12
Obsidian....
Grap. Dis.
Standards
Summary
For Help, press F1
Obsidian.devm:3
The Calibration Toolbox has the access points for all options. It is also how you navigate through your elements. The red forward > and backwards < buttons can be used to navigate between elements. You can set priorities for which fluorescence line you use (the numbers to the right
17 OBS_017_So... 0.04360 -0.01132 -26
18 OBS_018_So... 0.02030 -0.00091 -4.5
19 OBS_019_So... 0.02290 0.00158 6.9
20 OBS_020_So... 0.00110 0.00003 2.7
21 OBS_021_So... 0.01550 0.01565 0.00015 0.96
22 OBS_022_So... 0.03380 0.03227 -0.00153 -4.5
23 OBS_023_So... -6.0
24 OBS_024_So... -0.85
25 OBS_025_So... -17
26 OBS_026_So... 3.3
27 OBS_027_So... 8.4
28 OBS_028_So... 8.8
29 OBS_029_So... 7.0
30 OBS_030_So... -3.3
31 OBS_031_So... 10.0
32 OBS_032_So... 2.5
33 OBS_033_So... 2.3
34 OBS_034_So... 3.3
35 OBS_035_So... 3.2
36 OBS_036_So... 6.3
37 OBS_037_So... 8.2
38 OBS_038_So... 8.3
39 OBS_039_So... 5.0
40 OBS_040_So... 4.6
Calibration Toolbox
Rb
Rb KA1/Obsidian
1
2
3
Std Dev: 0.0022 %
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Double-click :enable or disable standard.
Squared correlation coefficient: 0.942596
Disable traces
Invert selection
->PPM
Status
10:48 AM
5/1/18

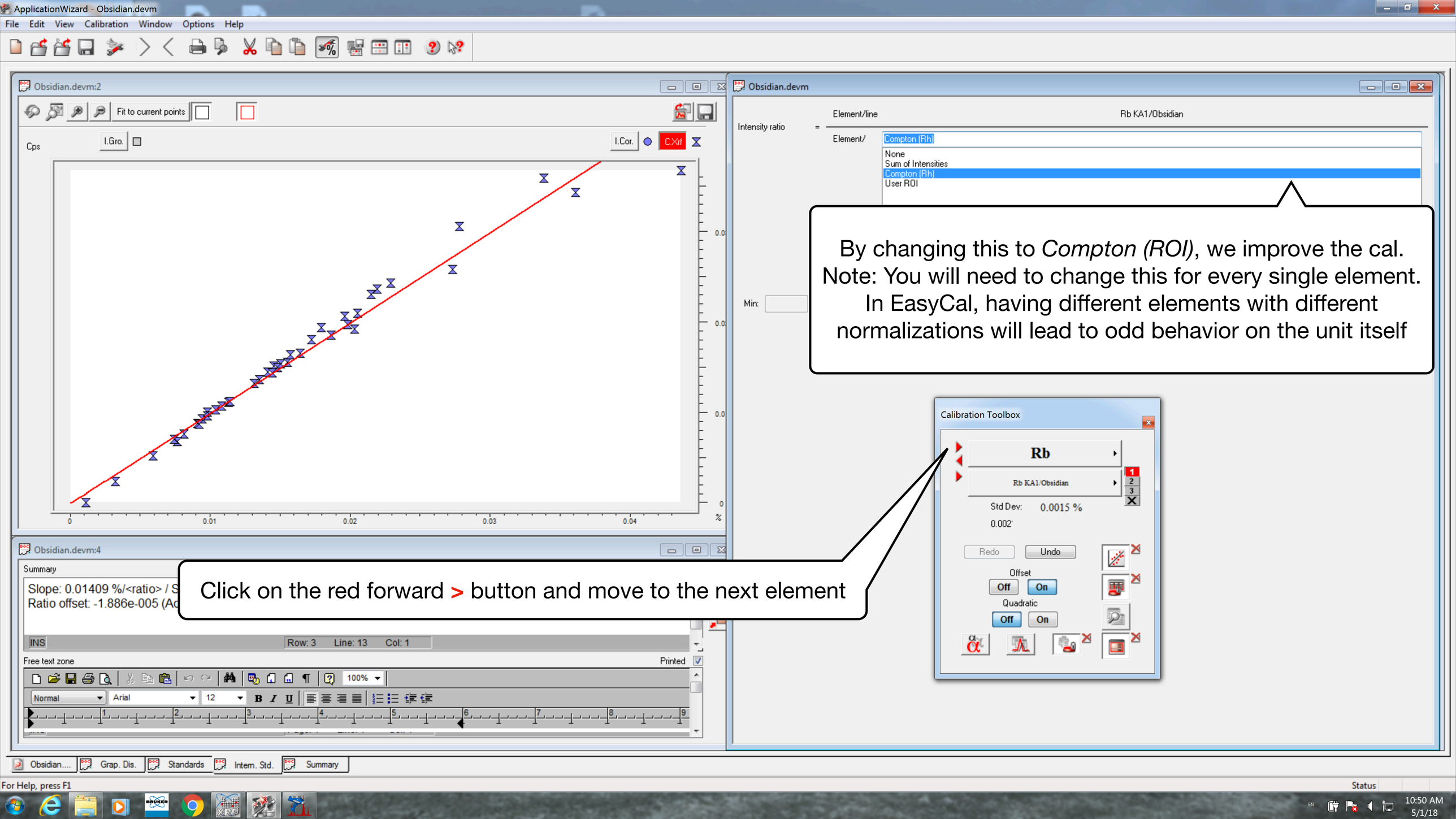

ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
C.Xrf
0.03
0.02
0.01
0
0.01
0.02
0.03
0.04
%
Obsidian.devm:3
Numbe\ Standard Name Chemical Concentration XRF Concentration Absolute Deviation Relative Deviation
1 OBS_001_So... 0.01720 0.01926 0.00206 12
2 OBS_002_So... 0.00910 0.01015 0.00105 12
3 OBS_003_So... 0.00940 0.01022 0.00082 8.7
4 OBS_004_So... 0.00590 0.00568 -0.00022 -3.7
5 OBS_005_So... 0.00320 0.00396 0.00076 24
6 OBS_006_So... 0.02730 0.02923 0.00193 7.1
7 OBS_007_So... 0.01790 0.01985 0.00195 11
17 OBS_017_So... 0.04360 0.03228 -0.01132 -26
18 OBS_018_So... 0.02030 0.01939 -0.00091 -4.5
19 OBS_019_So... 0.02290 0.02448 0.00158 6.9
20 OBS_020_So... 0.00110 0.00113 0.00003 2.7
21 OBS_021_So... 0.01550 0.01565 0.00015 0.96
22 OBS_022_So... 0.03380 0.03227 -0.00153 -4.5
23 OBS_023_So... -6.0
24 OBS_024_So... -0.85
25 OBS_025_So... -17
26 OBS_026_So... 3.3
27 OBS_027_So... 8.4
28 OBS_028_So... 8.8
29 OBS_029_So... 7.0
30 OBS_030_So... -3.3
31 OBS_031_So... 10.0
32 OBS_032_So... 2.5
33 OBS_033_So... 2.3
34 OBS_034_So... 3.3
35 OBS_035_So... 3.2
36 OBS_036_So... 6.3
37 OBS_037_So... 8.2
38 OBS_038_So... 8.3
39 OBS_039_So... 5.0
40 OBS_040_So... 4.6
Calibration Toolbox
Rb
Rb KA1/Obsidian
Std Dev: 0.0022 %
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Double-click :enable or disable standard.
Squared correlation coefficient: 0.942596
Disable traces
Invert selection
->PPM
The principle window you will need to keep an eye on is the Graph Display, which shows the validation curve of your calibration
Obsidian.devm:4
Summary
Printed
Squared correlation coefficient: 0.942596
Slope: 0.0007108 %/Cps / Sensitivity: 1407 Cps/% (Adjustable by regression)
INS
Row: 3 Line: 12 Col: 1
Free text zone
Printed
100%
Normal
Arial
12
Obsidian....
Grap. Dis.
Standards
Summary
For Help, press F1
Status
10:48 AM
5/1/18

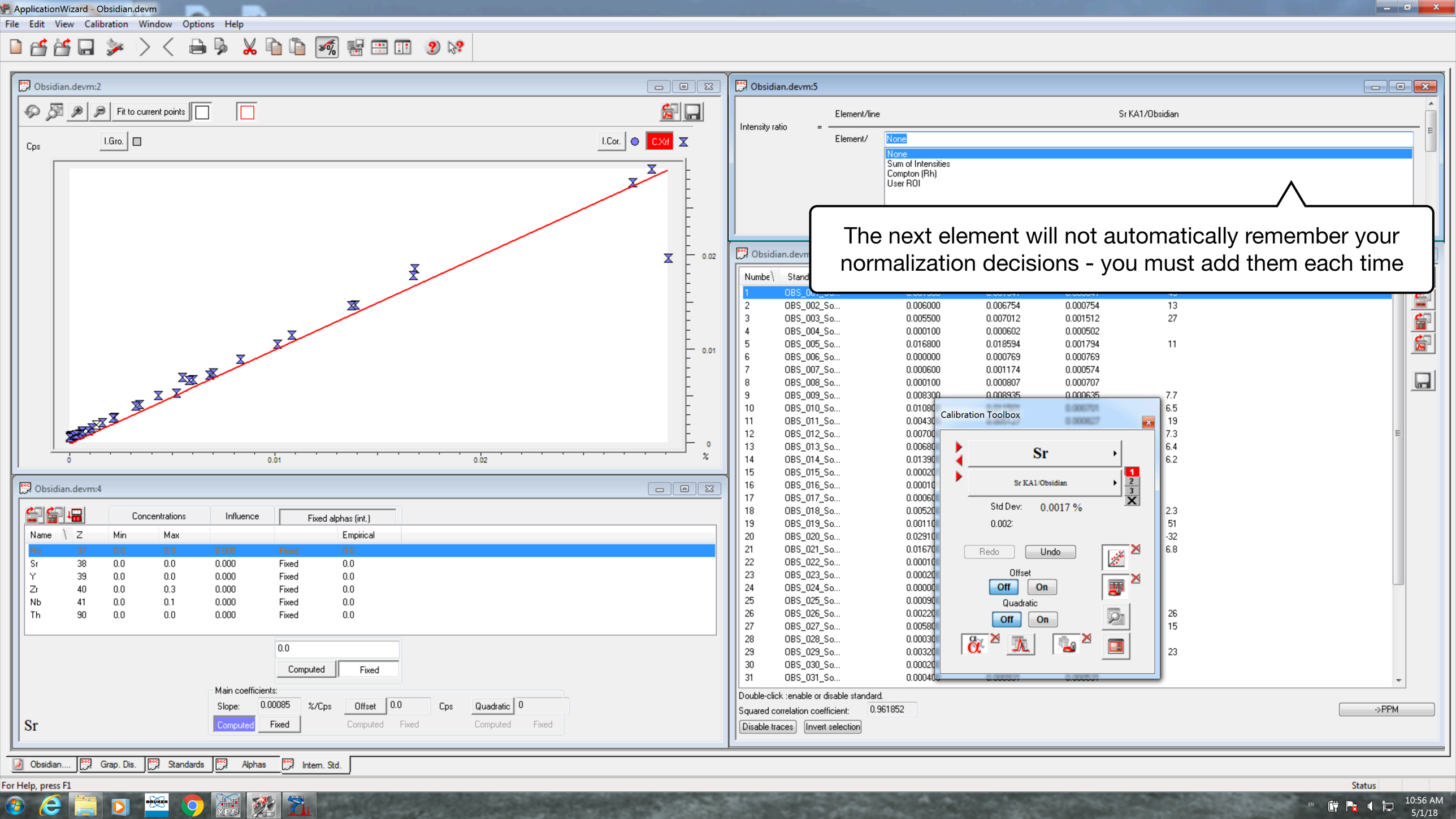


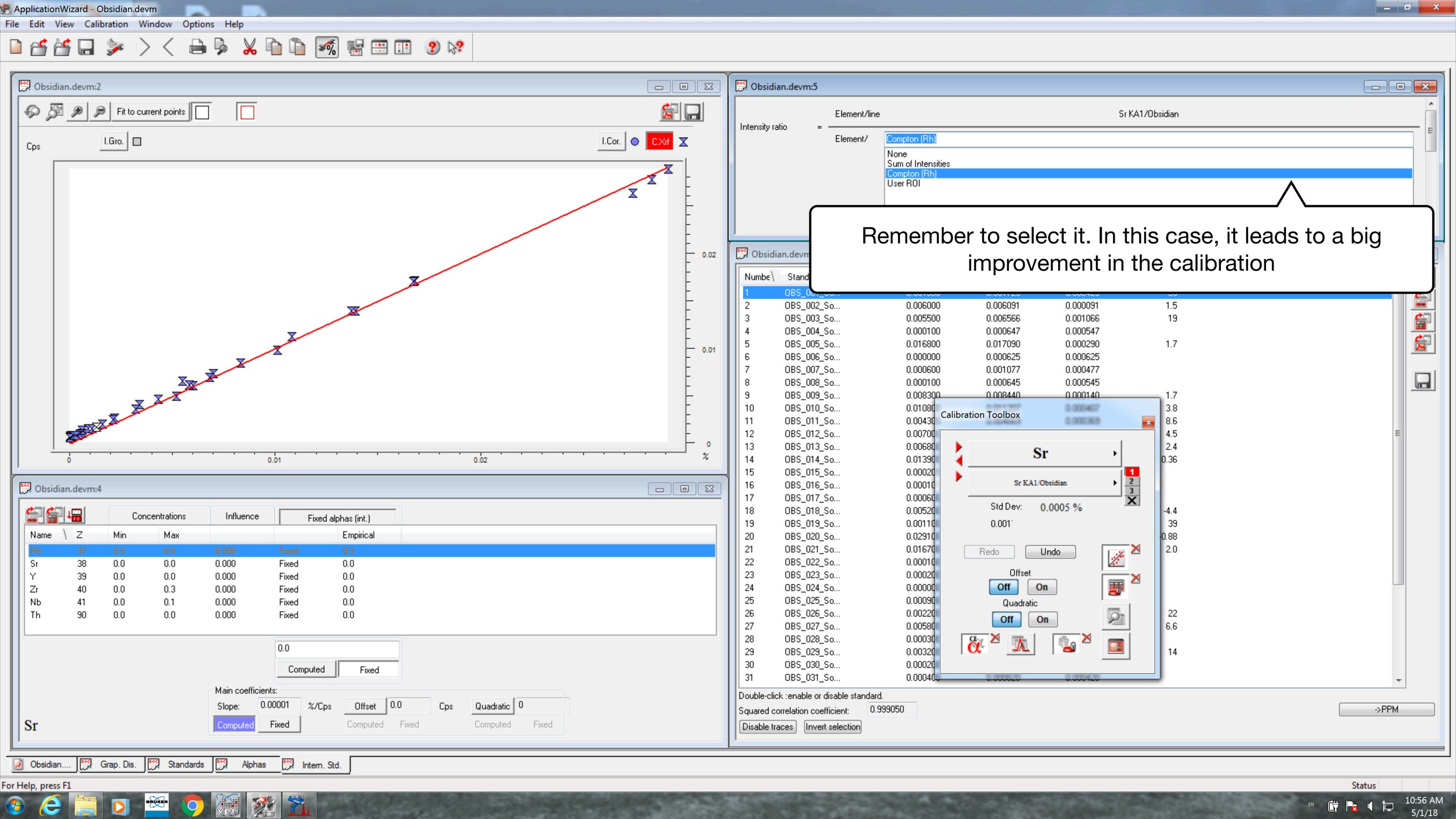
The Standards box shows each standard and its performance in the cal. At the bottom, you can see the R^2 (squared correlation coefficient)

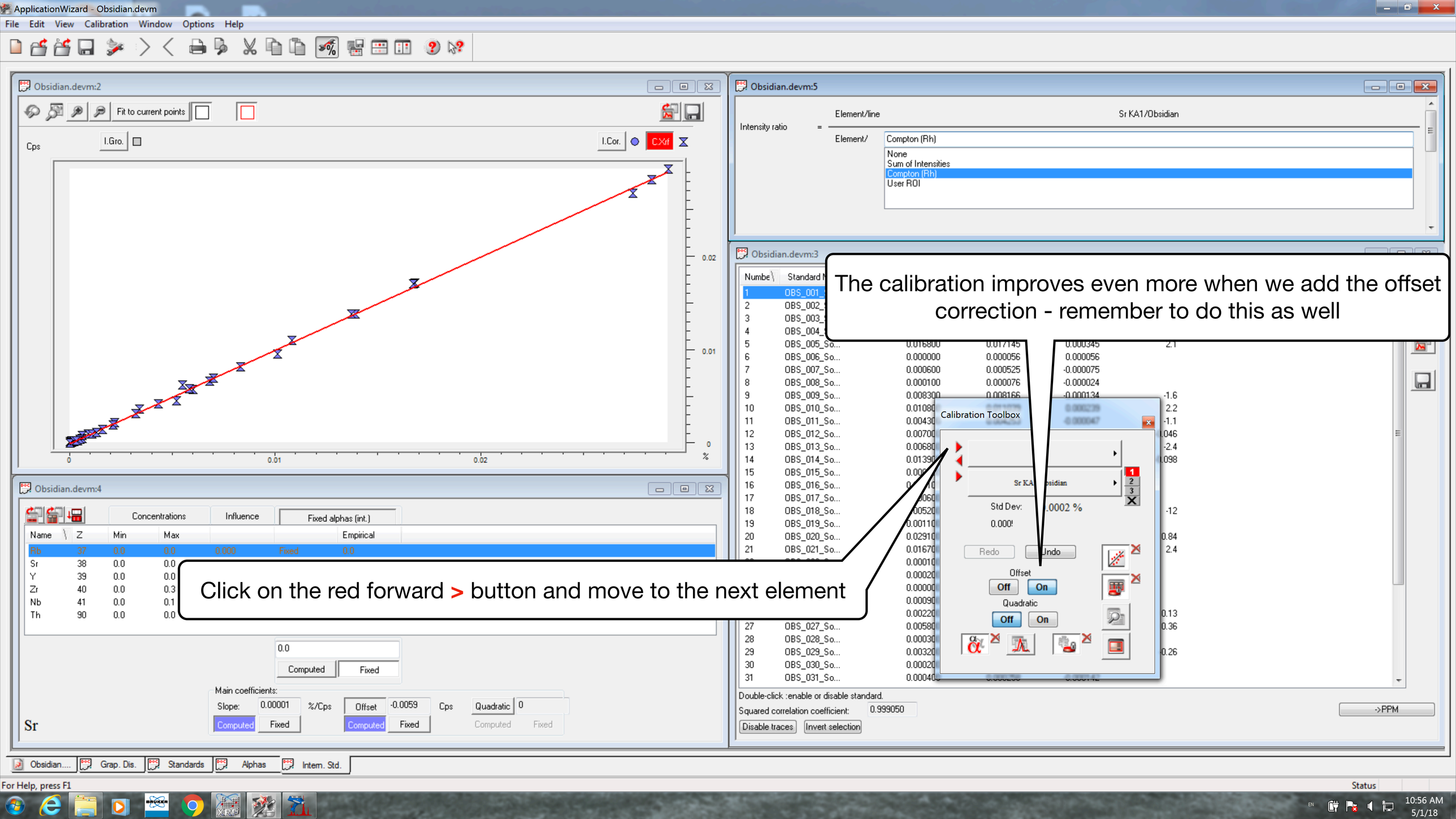

ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
Obsidian.devm:3
Numbe\ Standard Name Chemical Concentration XRF Concentration Absolute Deviation Relative Deviation
1 OBS_001_So... 0.01720 0.01921 0.00201 12
11 OBS_011_So... 0.00980 0.01036 0.00056 5.7
12 OBS_012_So... 0.01410 0.01405 -0.00005 -0.32
13 OBS_013_So... 0.01350 0.01352 0.00002 0.12
14 OBS_014_So... 0.00810 0.00801 -0.00009 -1.1
15 OBS_015_So... 0.00980 0.00977 -0.00003 -0.26
16 OBS_016_So... 0.01570 0.01552 -0.00018 -1.1
17 OBS_017_So... 0.04360 0.03295 -0.01065 -24
18 OBS_018_So... 0.02030 0.01935 -0.00095 -4.7
19 OBS_019_So... 0.02290 0.02472 0.00182 8.0
20 OBS_020_So... 0.00110 0.00009 -0.00101
21 OBS_021_So... 0.01550 0.01540 -0.00010 -0.62
22 OBS_022_So... 0.03380 0.03294 -0.00086 -2.5
23 OBS_023_So... -6.2
24 OBS_024_So... -0.45
25 OBS_025_So... -18
26 OBS_026_So... -1.6
27 OBS_027_So... 4.2
28 OBS_028_So... 7.4
29 OBS_029_So... 0.87
30 OBS_030_So... -3.5
31 OBS_031_So... 8.3
32 OBS_032_So... 0.71
33 OBS_033_So... 3.9
34 OBS_034_So... 2.3
35 OBS_035_So... -0.84
36 OBS_036_So... 6.5
37 OBS_037_So... 5.7
38 OBS_038_So... -0.72
39 OBS_039_So... -3.7
40 OBS_040_So... 5.2
To begin, add the Offset correction. I recommend doing this for all elements, but evaluate its effect, there may be some cases that this correction is not desirable
Calibration Toolbox
Std Dev:
No significant improvement.
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Double-click :enable or disable standard.
Squared correlation coefficient: 0.942596
Disable traces
Invert selection
->PPM
Obsidian.devm:4
Summary
Printed
Slope: 0.0007499 %/Cps / Sensitivity: 1334 Cps/% (Adjustable by regression)
Corrected intensity offset: -0.01106 Cps (Adjustable by regression) or 0.1 PPM
INS Row: 3 Line: 13 Col: 1
Free text zone
Printed
Normal
Arial
12
Obsidian.... Grap. Dis. Standards Summary
For Help, press F1
Status
10:50 AM
5/1/18


Our cal currently defaults to no normalization (which effectively means a time-based normalization)
When working with higher voltage ranges (30 - 50 kV) it may make sense to change to Compton normalization, click on the *Internal Standard* button to reveal the window
ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Obsidian.devm
Element/line
Rb KA1/Obsidian
Element/
None
Sum of Intensities
Compton (Rh)
User ROI
Min:
keV
Max:
keV
Cps
I.Gro.
Calibration Toolbox
Rb
Rb KA1/Obsidian
Std Dev: 0.0021 %
0.002
No significant improvement.
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian.devm:4
Summary
Slope: 0.0007499 %/Cps / Sensitivity: 1334 Cps/%
Corrected intensity offset: -0.01106 Cps (Adjustable by regression) or 0.1 PPM
INS
Row: 3 Line: 13 Col: 1
Free text zone
Printed
Normal
Arial
12
Obsidian....
Grap. Dis.
Standards
Intern. Std.
Summary
For Help, press F1
Status
10:50 AM
5/1/18


ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
Obsidian.devm
Element/line
Rb KA1/Obsidian
Intensity ratio
Element/
Compton (Rb)
None
Sum of Intensities
Compton (Rb)
User ROI
Min:
By changing this to Compton (ROI), we improve the cal.
Note: You will need to change this for every single element.
In EasyCal, having different elements with different normalizations will lead to odd behavior on the unit itself
Calibration Toolbox
Rb
Rb KA1/Obsidian
Std Dev: 0.0015 %
0.002
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian.devm:4
Summary
Slope: 0.01409 %/<ratio> / S
Ratio offset: -1.886e-005 (Ac
INS
Row: 3 Line: 13 Col: 1
Free text zone
Printed
100%
Normal
Arial
12
Click on the red forward > button and move to the next element
Obsidian....
Grap. Dis.
Standards
Intern. Std.
Summary
For Help, press F1
Status
10:50 AM
5/1/18


ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
0.02
0.01
0
0
0.01
0.02
%
Obsidian.devm:5
Intensity ratio
=
Element/line
Sr KA1/Obsidian
Element/
None
None
Sum of Intensities
Compton (Rh)
User ROI
The next element will not automatically remember your normalization decisions - you must add them each time
Obsidian.devm:4
Concentrations
Influence
Fixed alphas (int.)
Name \ Z Min Max Empirical
Rb 37 0.0 0.0 0.000 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Fixed 0.0
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
0.0
Computed
Fixed
Main coefficients:
Slope: 0.00085 %/Cps
Offset 0.0 Cps
Quadratic 0
Computed Fixed
Computed Fixed
Computed Fixed
Sr
Numbe\ Stand
1 OBS_0...
2 OBS_002_So... 0.006000 0.006754 0.000754 13
3 OBS_003_So... 0.005500 0.007012 0.001512 27
4 OBS_004_So... 0.000100 0.000602 0.000502
5 OBS_005_So... 0.016800 0.018594 0.001794 11
6 OBS_006_So... 0.000000 0.000769 0.000769
7 OBS_007_So... 0.000600 0.001174 0.000574
8 OBS_008_So... 0.000100 0.000807 0.000707
9 OBS_009_So... 0.008300 0.008935 0.000635 7.7
10 OBS_010_So... 0.01080 6.5
11 OBS_011_So... 0.00430 19
12 OBS_012_So... 0.00700 7.3
13 OBS_013_So... 0.00680 6.4
14 OBS_014_So... 0.01390 6.2
15 OBS_015_So... 0.00020
16 OBS_016_So... 0.00010
17 OBS_017_So... 0.00060
18 OBS_018_So... 0.00520 2.3
19 OBS_019_So... 0.00110 51
20 OBS_020_So... 0.02910 -32
21 OBS_021_So... 0.01670 6.8
22 OBS_022_So... 0.00010
23 OBS_023_So... 0.00020
24 OBS_024_So... 0.00000
25 OBS_025_So... 0.00090
26 OBS_026_So... 0.00220 26
27 OBS_027_So... 0.00580 15
28 OBS_028_So... 0.00030
29 OBS_029_So... 0.00320 23
30 OBS_030_So... 0.00020
31 OBS_031_So... 0.00040
Double-click :enable or disable standard.
Squared correlation coefficient: 0.961852
Disable traces
Invert selection
->PPM
Calibration Toolbox
Sr
Sr KA1/Obsidian
1
2
3
Std Dev: 0.0017 %
0.002:
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian....
Grap. Dis.
Standards
Alphas
Intern. Std.
For Help, press F1
Status
10:56 AM
5/1/18


ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
0.02
0.01
0
%
Obsidian.devm:5
Intensity ratio =
Element/line
Sr KA1/Obsidian
Element/
Compton (Rh)
None
Sum of Intensities
Compton (Rh)
User ROI
Remember to select it. In this case, it leads to a big improvement in the calibration
Obsidian.devm:4
Concentrations
Influence
Fixed alphas (int.)
Name Z Min Max Empirical
Rb 37 0.0 0.0 0.000 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Fixed 0.0
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
Computed
Fixed
Main coefficients:
Slope: 0.00001 %/Cps
Offset 0.0 Cps
Quadratic 0
Sr
Calibration Toolbox
Sr
Sr KA1/Obsidian
Std Dev: 0.0005 %
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Double-click :enable or disable standard.
Squared correlation coefficient: 0.999050
Disable traces
Invert selection
->PPM
Obsidian....
Grap. Dis.
Standards
Alphas
Intern. Std.
For Help, press F1
Status
10:56 AM
5/1/18


ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
0.02
0.01
0
%
Obsidian.devm:5
Intensity ratio
Element/line
Sr KA1/Obsidian
Element/
Compton (Rh)
None
Sum of Intensities
Compton (Rh)
User ROI
Obsidian.devm:3
Numbe
Standard
1 OBS_001_
2 OBS_002_
3 OBS_003_
4 OBS_004_
5 OBS_005_So...
6 OBS_006_So...
7 OBS_007_So...
8 OBS_008_So...
9 OBS_009_So...
10 OBS_010_So...
11 OBS_011_So...
12 OBS_012_So...
13 OBS_013_So...
14 OBS_014_So...
15 OBS_015_So...
16 OBS_016_So...
17 OBS_017_So...
18 OBS_018_So...
19 OBS_019_So...
20 OBS_020_So...
21 OBS_021_So...
27 OBS_027_So...
28 OBS_028_So...
29 OBS_029_So...
30 OBS_030_So...
31 OBS_031_So...
Calibration Toolbox
Std Dev:
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Double-click :enable or disable standard.
Squared correlation coefficient:
0.999050
Disable traces
Invert selection
->PPM
Obsidian.devm:4
Concentrations
Influence
Fixed alphas (int.)
Name
Z
Min
Max
Empirical
Rb 37 0.0 0.0 0.000 Fixed 0.0
Sr 38 0.0 0.0
Y 39 0.0 0.0
Zr 40 0.0 0.3
Nb 41 0.0 0.1
Th 90 0.0 0.0
0.0
Computed
Fixed
Main coefficients:
Slope: 0.00001 %/Cps
Offset -0.0059 Cps
Quadratic 0
Computed
Fixed
Sr
The calibration improves even more when we add the offset correction - remember to do this as well
Click on the red forward > button and move to the next element
Obsidian....
Grap. Dis.
Standards
Alphas
Intern. Std.
For Help, press F1
Status
10:56 AM
5/1/18

ApplicationWizard - Obsidian.devm

File Edit View Calibration Window Options Help

Obsidian.devm:2

Fit to current points

Cps I.Gro. I.Cor. CXrf

0 0.01 0.02 0.03 0.04 %

0 0.01 0.02 0.03

Obsidian.devm:4

Concentrations Influence Fixed alphas (int.)

Name	Z	Min	Max			Empirical
Rb	37	0.0	0.0	0.000	Fixed	0.0
Sr	38	0.0	0.0	0.000	Fixed	0.0
Y	39	0.0	0.0	0.000	Fixed	0.0
Zr	40	0.0	0.3	0.000	Fixed	0.0
Nb	41	0.0	0.1	0.000	Fixed	0.0
Th	90	0.0	0.0	0.000	Fixed	0.0

0.0 Computed Fixed

Main coefficients:

Slope: 0.00002 %/Cps Computed Fixed

Offset -0.0299 Cps Computed Fixed

Quadratic 0 Computed Fixed

Y

Obsidian.devm:5

Intensity ratio = Element/line Y KA1/Obsidian

Element/ Compton (Rh)

None
Sum of Intensities
Compton (Rh)
User ROI

Obsidian.devm:3

For this element, the Compton normalization and offset corrections are not enough to make a good model

Nu				
1				
2				
3				
4				
5				
6	OBS_006_So...	0.02070	0.02109	0.00039	1.9
7	OBS_007_So...	0.00270	0.00344	0.00074	28
8	OBS_008_So...	0.00850	0.01021	0.00171	20
9	OBS_009_So...	0.00230	0.00167	-0.00063	-27
10	OBS_010_So...	0.0015			6.4
11	OBS_011_So...	0.0025			-41
12	OBS_012_So...	0.0025			8.0
13	OBS_013_So...	0.0026			.066
14	OBS_014_So...	0.0019			
15	OBS_015_So...	0.0077			9.3
16	OBS_016_So...	0.0070			12
17	OBS_017_So...	0.0415			-15
18	OBS_018_So...	0.0088			2.1
19	OBS_019_So...	0.0039			37
20	OBS_020_So...	0.0021			
21	OBS_021_So...	0.0039			0.94
22	OBS_022_So...	0.0118			26
23	OBS_023_So...	0.0101			13
24	OBS_024_So...	0.0171			19
25	OBS_025_So...	0.0136			5.9
26	OBS_026_So...	0.0053			-6.6
27	OBS_027_So...	0.0018			-42
28	OBS_028_So...	0.0042			2.3
29	OBS_029_So...	0.0050			-7.0
30	OBS_030_So...	0.0108			14
31	OBS_031_So...	0.0021			-7.5

Calibration Toolbox

Y KA1 idian

Std Dev: 0016 %

0.002

Redo Undo

Offset Off On

Quadratic Off On

Double-click :enable or disable standard.

Squared correlation coefficient: 0.953284

Disable traces Invert selection

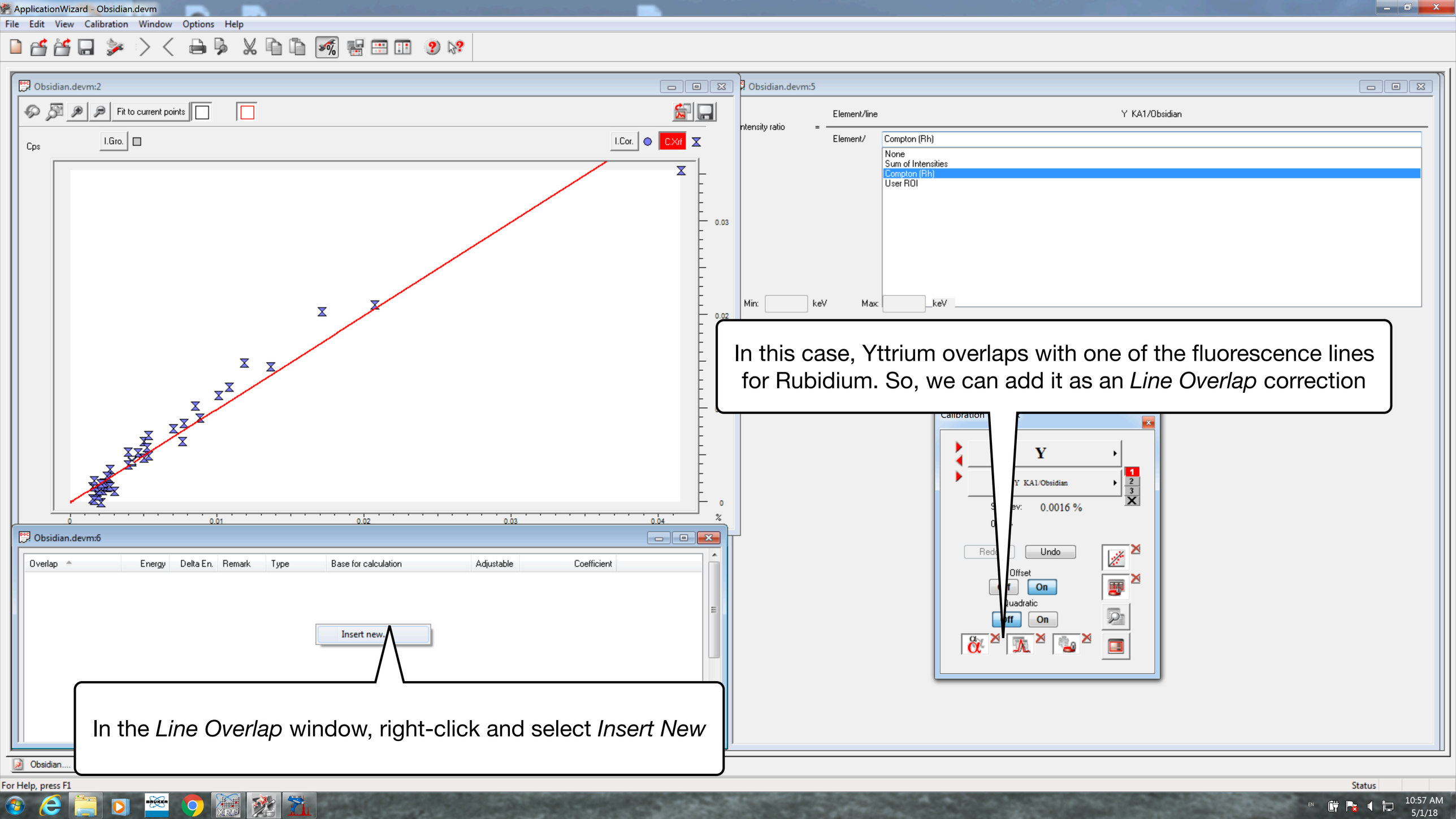
->PPM

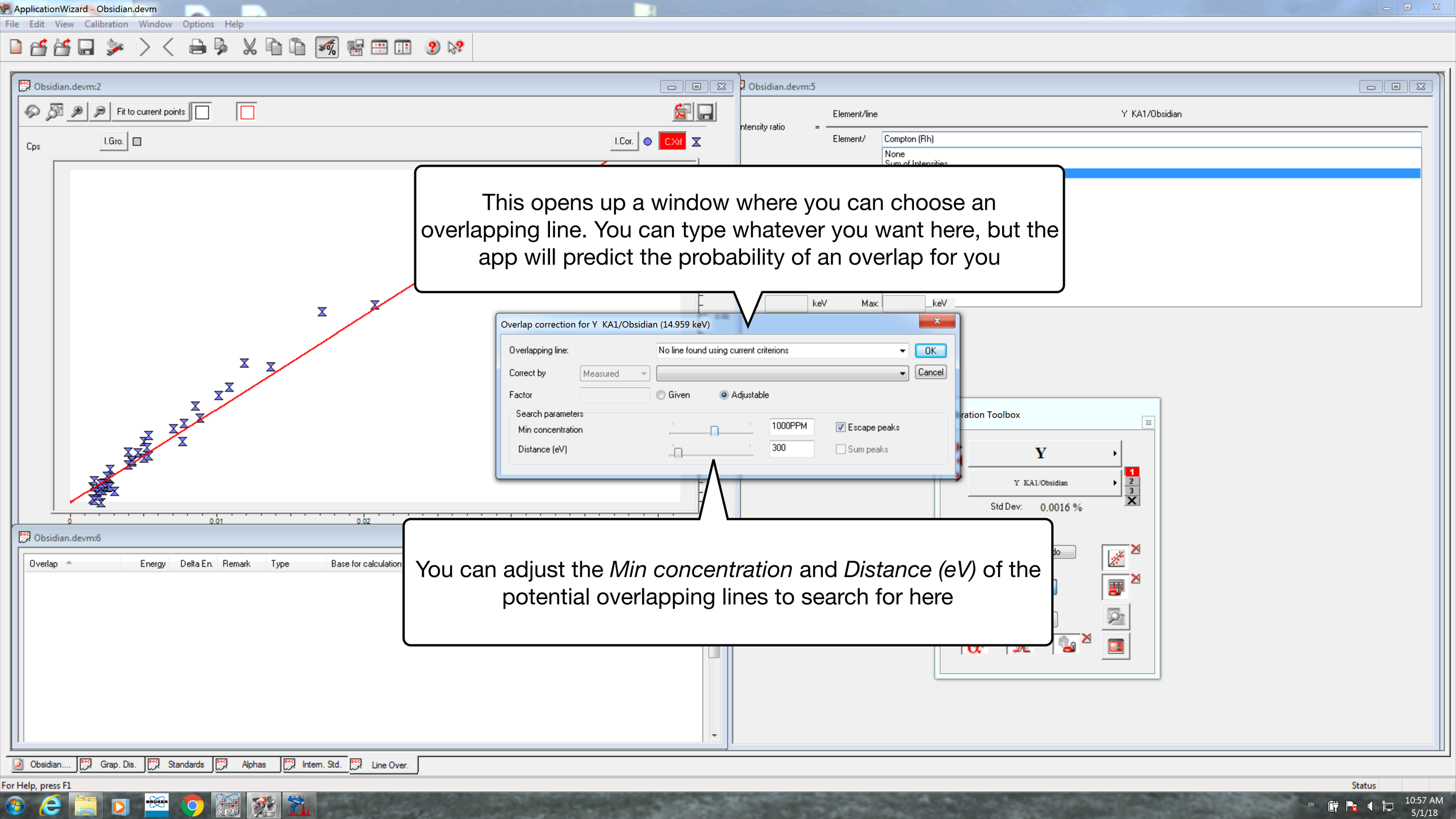
Obsidian.... Grap. Dis. Standards Alphas Intern. Std.

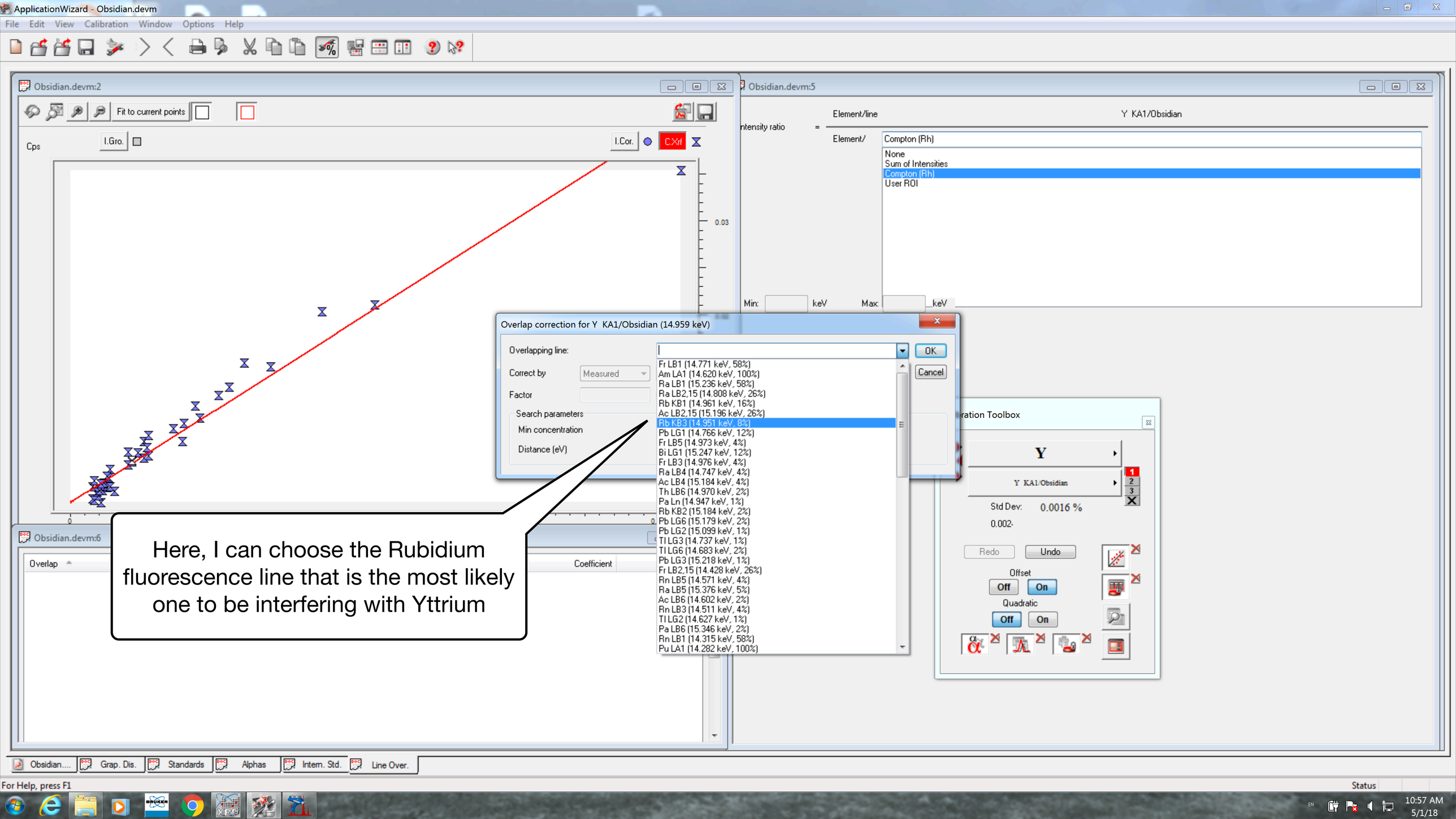
For Help, press F1

Status

10:56 AM 5/1/18


ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
0.03
0.02
0
0.01
0.02
0.03
0.04
%
Obsidian.devm:5
Element/line
Y KA1/Obsidian
Element/
Compton (Rh)
None
Sum of Intensities
Compton (Rh)
User ROI
Min:
keV
Max:
keV
Obsidian.devm:6
Overlap
Energy
Delta En.
Remark
Type
Base for calculation
Adjustable
Coefficient
Insert new...
In this case, Yttrium overlaps with one of the fluorescence lines for Rubidium. So, we can add it as an *Line Overlap* correction
Calibration
Y
Y KA1/Obsidian
0.0016 %
Undo
Offset
On
Quadratic
Off
On
In the *Line Overlap* window, right-click and select *Insert New*
For Help, press F1
Status
10:57 AM
5/1/18


This opens up a window where you can choose an overlapping line. You can type whatever you want here, but the app will predict the probability of an overlap for you
You can adjust the *Min concentration* and *Distance (eV)* of the potential overlapping lines to search for here
Overlap correction for Y KA1/Obsidian (14.959 keV)
Overlapping line:
No line found using current criterions
OK
Correct by
Measured
Cancel
Factor
Given
Adjustable
Search parameters
Min concentration
1000PPM
Escape peaks
Distance (eV)
300
Sum peaks
Obsidian.devm:2
Obsidian.devm:5
Obsidian.devm:6
Fit to current points
I.Gro.
I.Cor.
CXrf
Cps
Element/line
Y KA1/Obsidian
Compton (Rh)
None
Overlap
Energy
Delta En.
Remark
Type
Base for calculation
Std Dev: 0.0016 %
Obsidian....
Grap. Dis.
Standards
Alphas
Intern. Std.
Line Over.
For Help, press F1
Status


ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
0.03
Obsidian.devm:5
Element/line
Y KA1/Obsidian
Element/
Compton (Rh)
None
Sum of Intensities
Compton (Rh)
User ROI
Min:
keV
Max:
keV
Overlap correction for Y KA1/Obsidian (14.959 keV)
Overlapping line:
Correct by
Measured
Factor
Search parameters
Min concentration
Distance (eV)
OK
Cancel
Fr LB1 (14.771 keV, 58%)
Am LA1 (14.620 keV, 100%)
Ra LB1 (15.236 keV, 58%)
Ra LB2,15 (14.808 keV, 26%)
Rb KB1 (14.961 keV, 16%)
Ac LB2,15 (15.196 keV, 26%)
Rb KB3 (14.951 keV, 8%)
Pb LG1 (14.766 keV, 12%)
Fr LB5 (14.973 keV, 4%)
Bi LG1 (15.247 keV, 12%)
Fr LB3 (14.976 keV, 4%)
Ra LB4 (14.747 keV, 4%)
Ac LB4 (15.184 keV, 4%)
Th LB6 (14.970 keV, 2%)
Pa Ln (14.947 keV, 1%)
Rb KB2 (15.184 keV, 2%)
Pb LG6 (15.179 keV, 2%)
Pb LG2 (15.099 keV, 1%)
Tl LG3 (14.737 keV, 1%)
Tl LG6 (14.683 keV, 2%)
Pb LG3 (15.218 keV, 1%)
Fr LB2,15 (14.428 keV, 26%)
Rn LB5 (14.571 keV, 4%)
Ra LB5 (15.376 keV, 5%)
Ac LB6 (14.602 keV, 2%)
Rn LB3 (14.511 keV, 4%)
Tl LG2 (14.627 keV, 1%)
Pa LB6 (15.346 keV, 2%)
Rn LB1 (14.315 keV, 58%)
Pu LA1 (14.282 keV, 100%)
ration Toolbox
Y
Y KA1/Obsidian
Std Dev: 0.0016 %
0.002
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian.devm:6
Overlap
Coefficient
Here, I can choose the Rubidium fluorescence line that is the most likely one to be interfering with Yttrium
Obsidian....
Grap. Dis.
Standards
Alphas
Intern. Std.
Line Over.
For Help, press F1
Status
10:57 AM
5/1/18

ApplicationWizard - Obsidian.devm

File Edit View Calibration Window Options Help

Obsidian.devm:2

Fit to current points

Cps I.Gro. I.Cor. CXrf

0.03 0.02 0.01

0 0.01 0.03 0.04 %

Obsidian.devm:5

Element/line Y KA1/Obsidian

Intensity ratio = Element/ Compton (Rh)

None
Sum of Intensities
Compton (Rh)
User ROI

This element's calibration requires more work - this is an instance where slope corrections would be helpful. Click on the *Alphas* button

Calibration Tool

Y

A1/Obsidian

1 2 3

Std D 0.0013 %

0.001

Redo Undo

Off On

Quadratic

Off On

The correction is now listed in the *Line Overlap* window

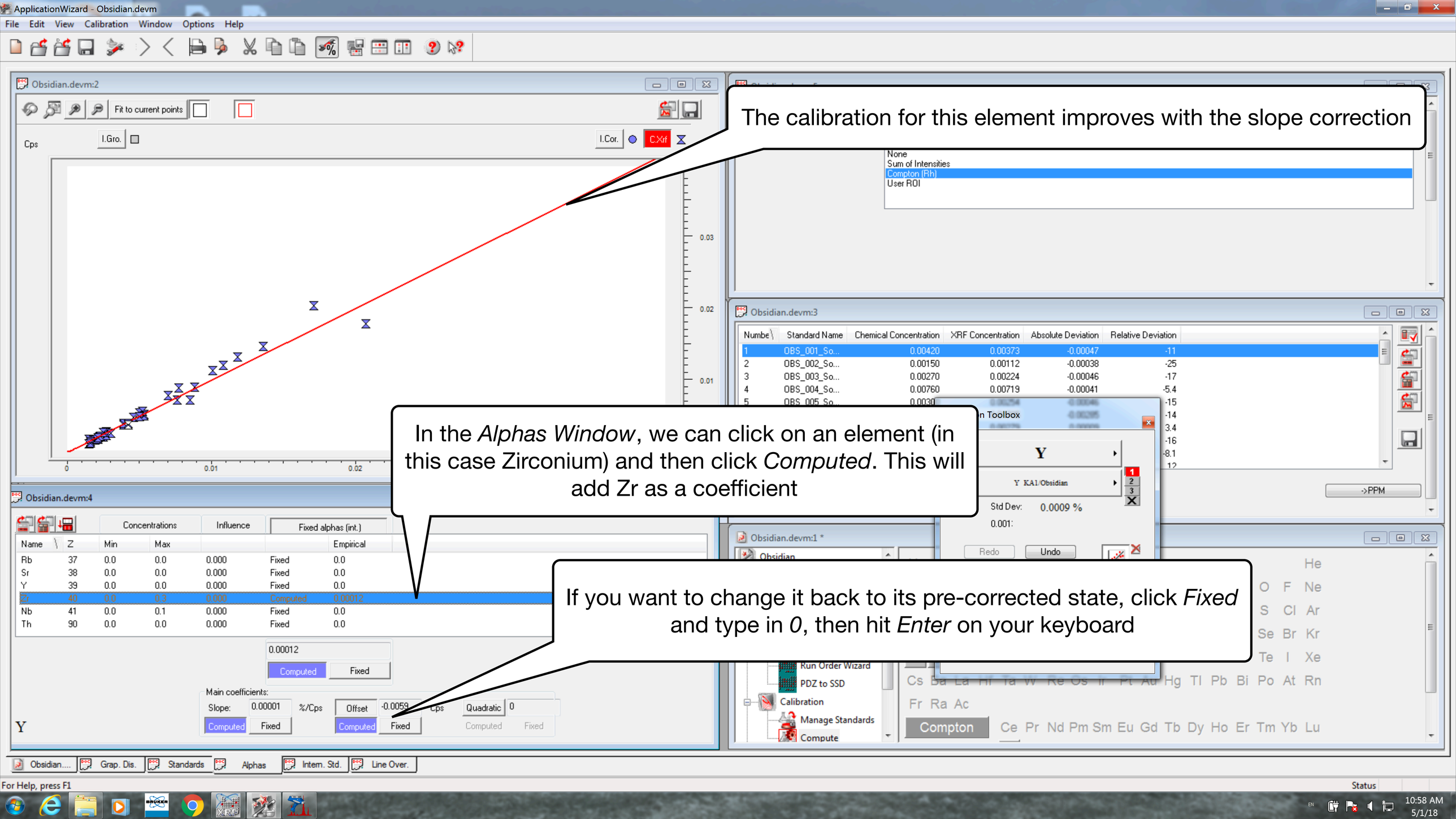
Obsidian.devm:6

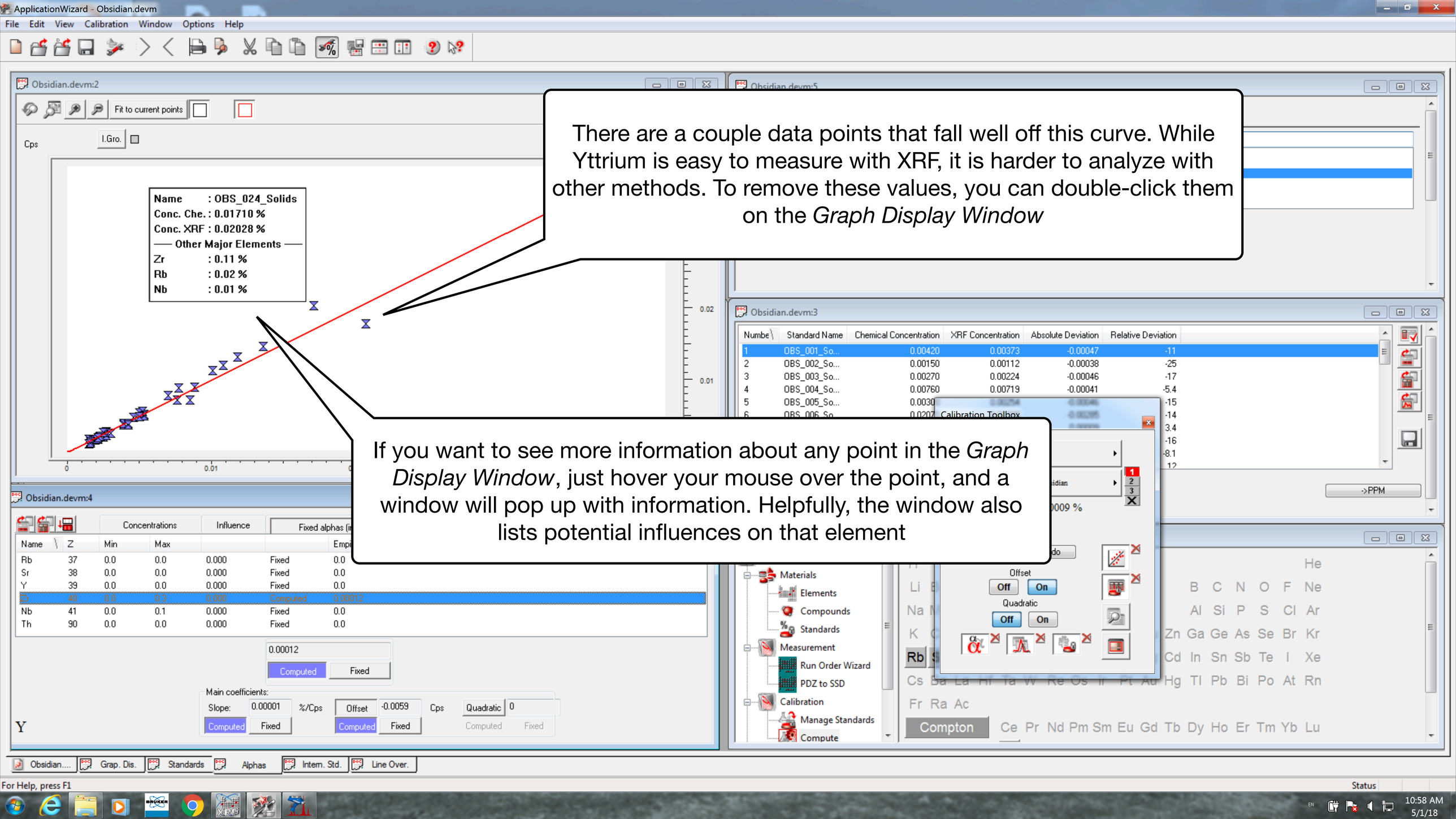
Overlap	Energy	Delta En.	Remark	Type	Base for calculation	Adjustable	Coefficient
Rb KB3	14.951	0.008		Measured	Rb KA1/Obsidian	Adjustable	-6.986e-007

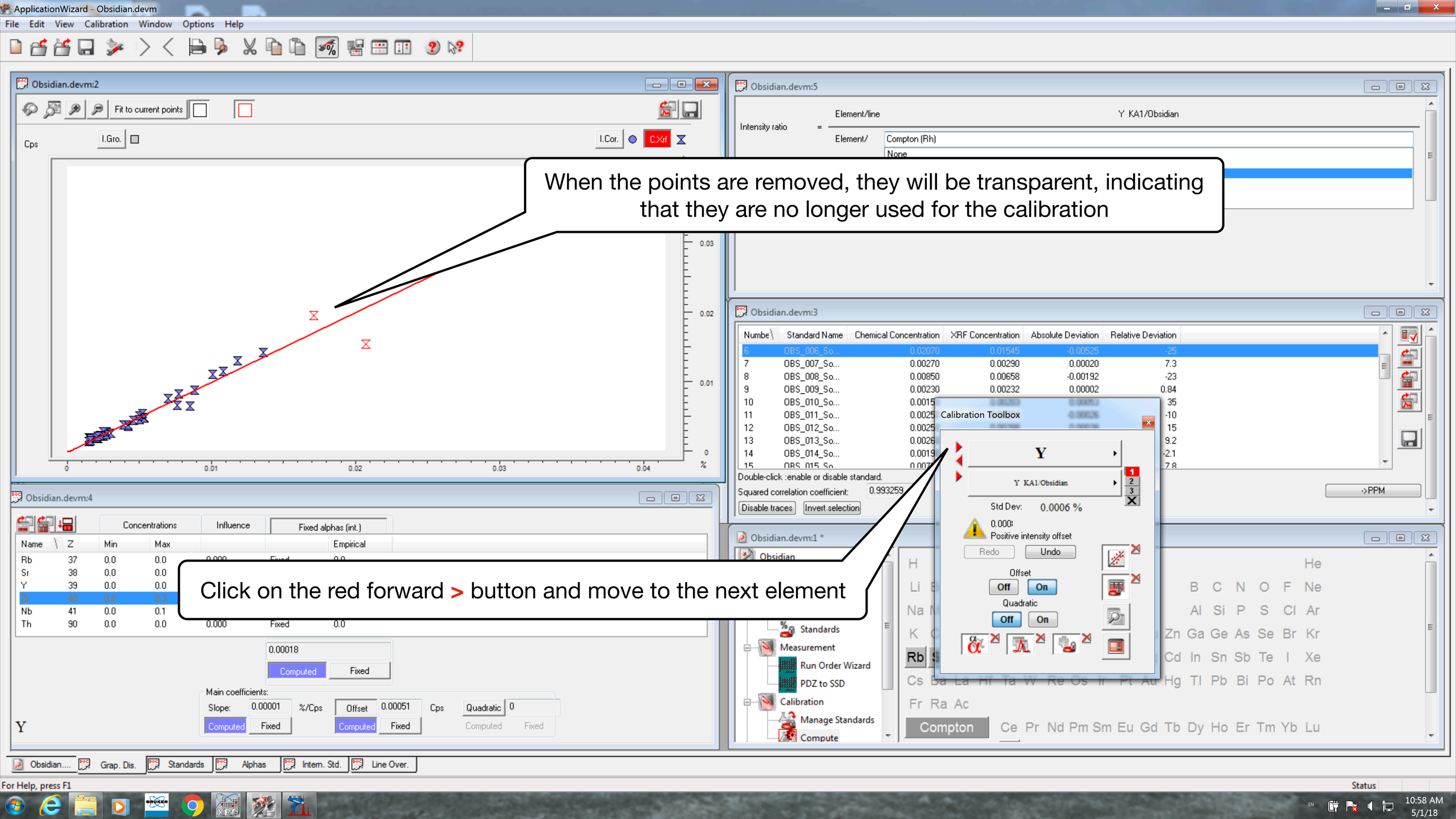
Obsidian.... Grap. Dis. Standards Alphas Intern. Std. Line Over.

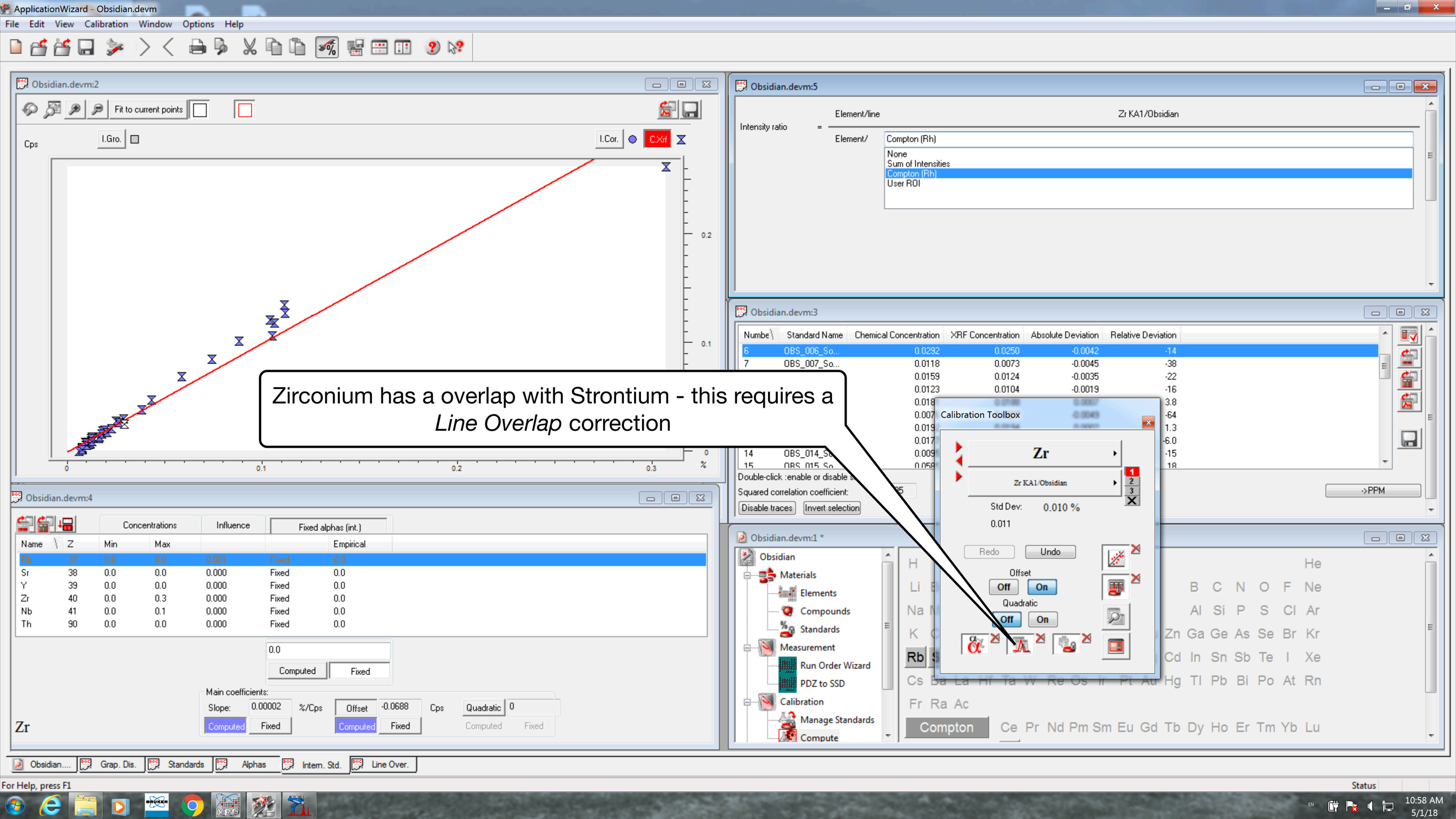
For Help, press F1 Status

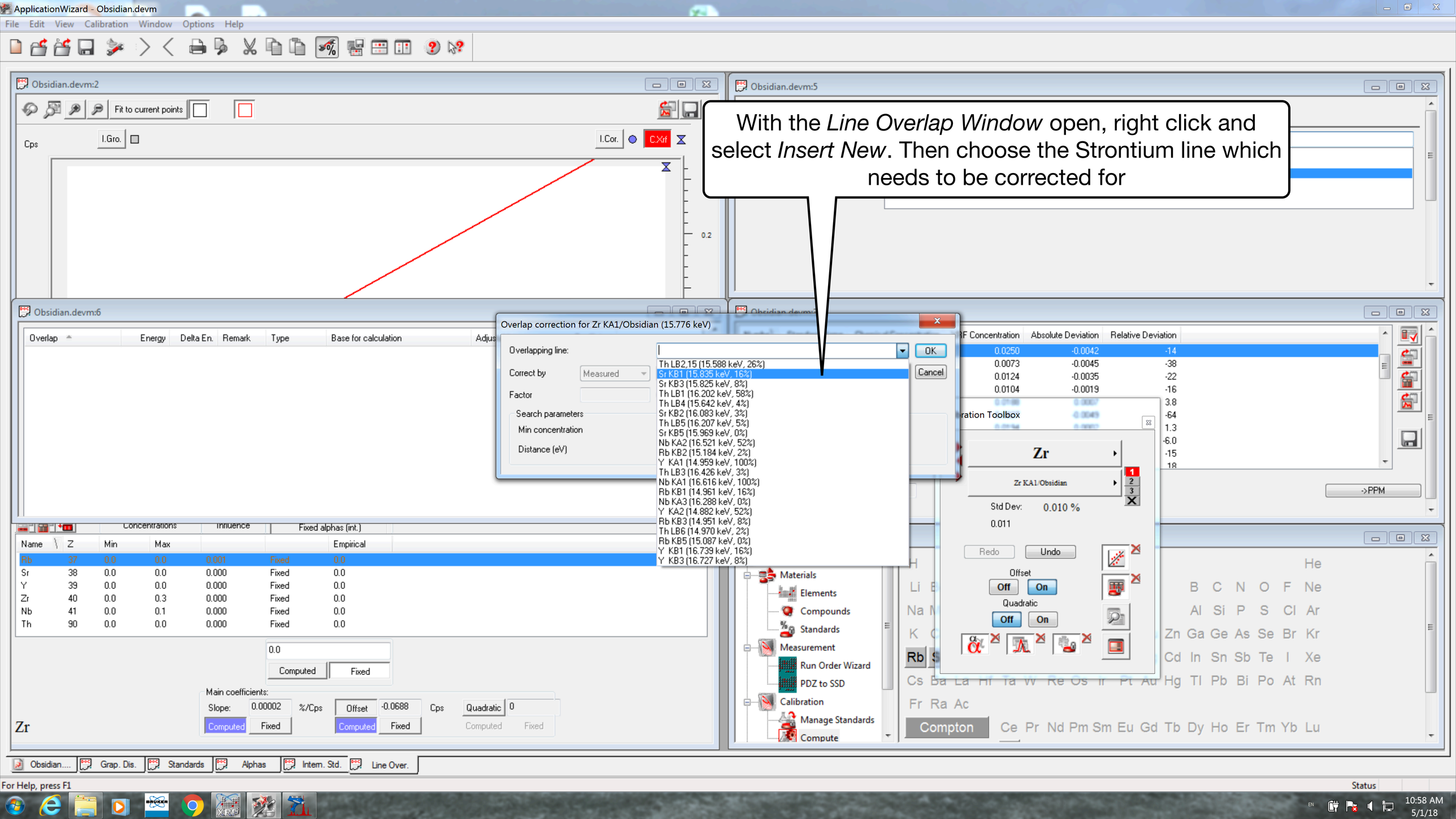
10:57 AM 5/1/18

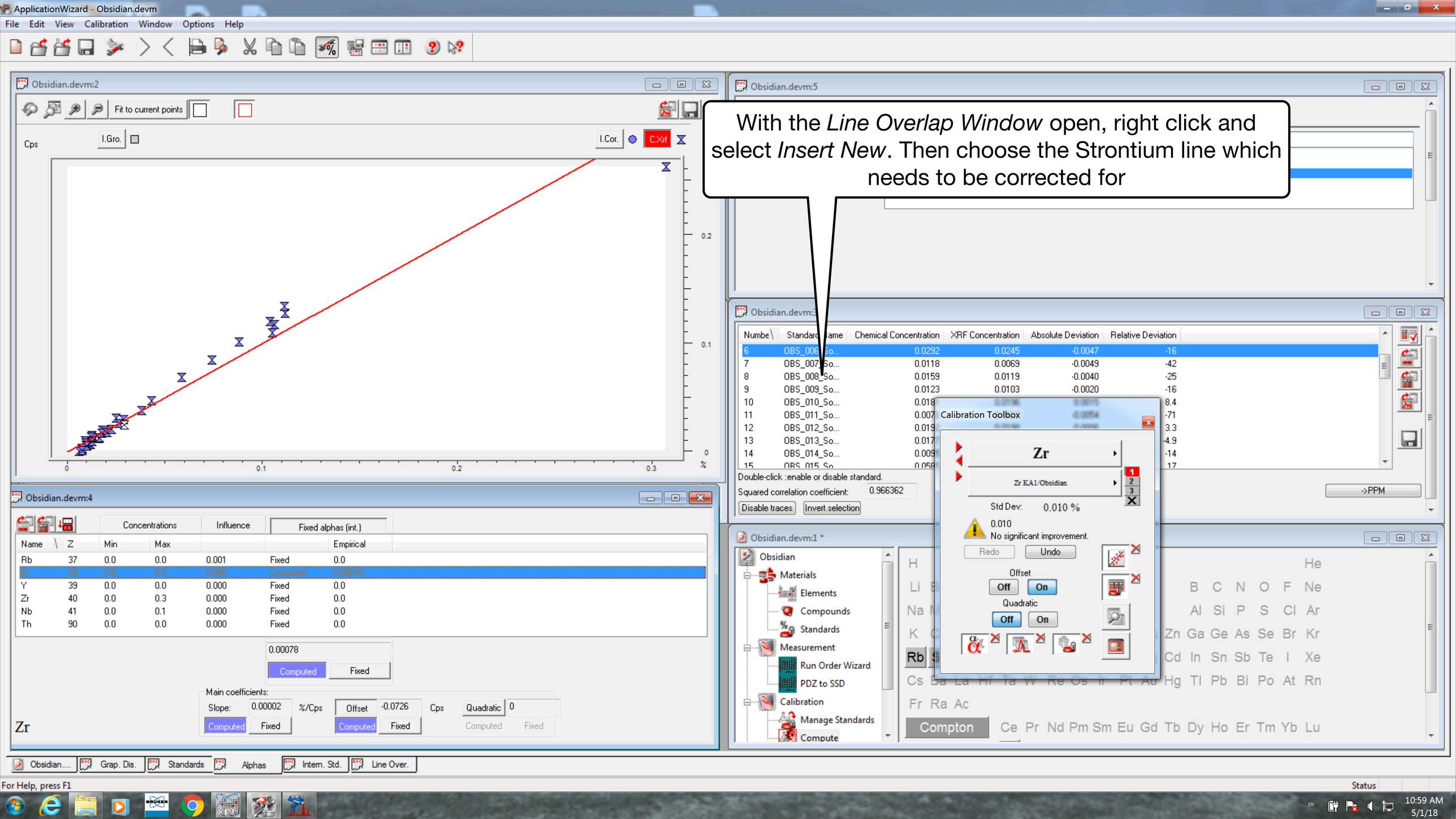

The calibration for this element improves with the slope correction
In the *Alphas Window*, we can click on an element (in this case Zirconium) and then click *Computed*. This will add Zr as a coefficient
If you want to change it back to its pre-corrected state, click *Fixed* and type in *0*, then hit *Enter* on your keyboard

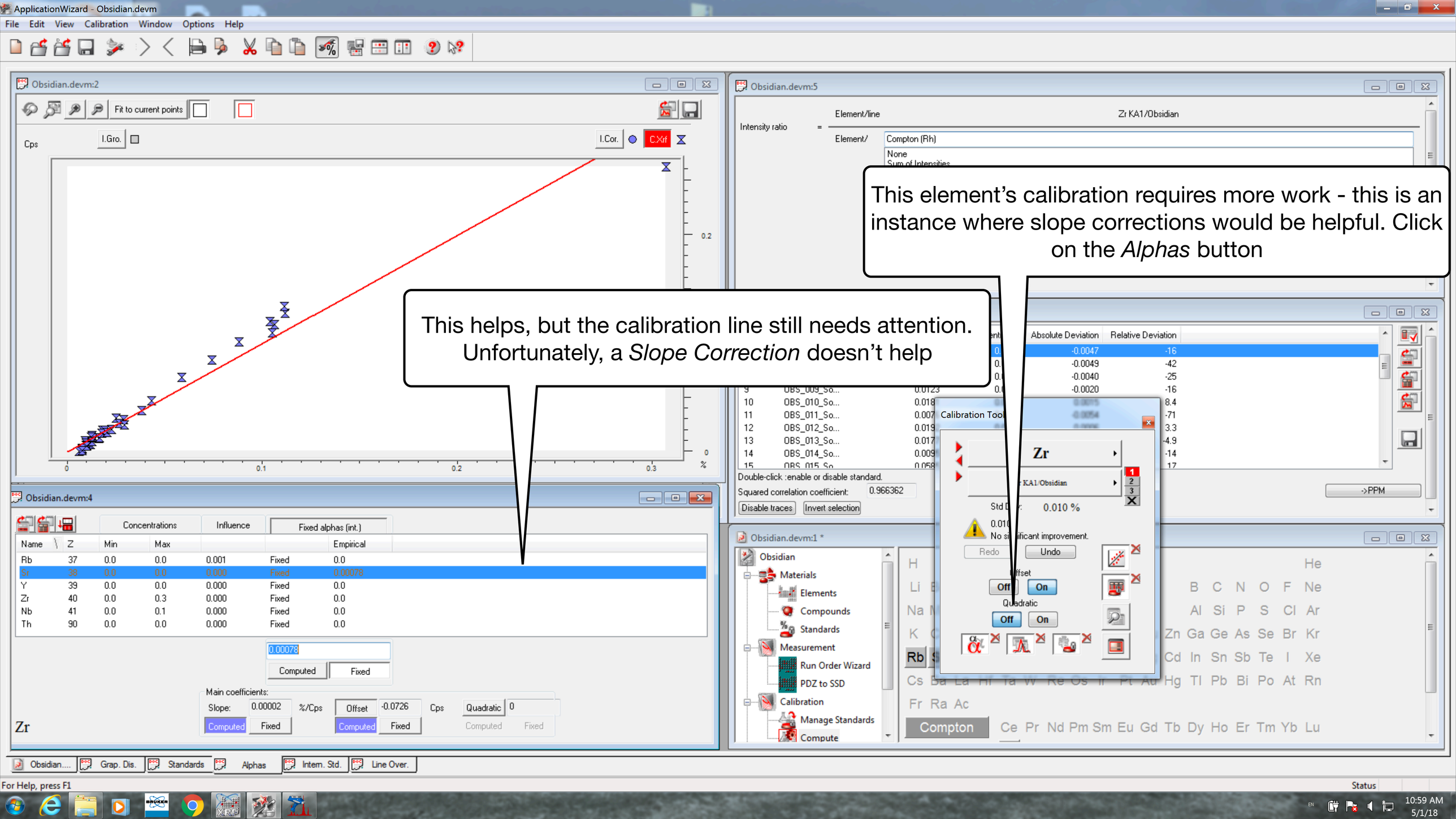

There are a couple data points that fall well off this curve. While Yttrium is easy to measure with XRF, it is harder to analyze with other methods. To remove these values, you can double-click them on the *Graph Display Window*
If you want to see more information about any point in the *Graph Display Window*, just hover your mouse over the point, and a window will pop up with information. Helpfully, the window also lists potential influences on that element
ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
I.Gro.
Cps
Name : OBS_024_Solids
Conc. Che. : 0.01710 %
Conc. XRF : 0.02028 %
Other Major Elements
Zr : 0.11 %
Rb : 0.02 %
Nb : 0.01 %
Obsidian.devm:3
Numbe Standard Name Chemical Concentration XRF Concentration Absolute Deviation Relative Deviation
1 OBS_001_So... 0.00420 0.00373 -0.00047 -11
2 OBS_002_So... 0.00150 0.00112 -0.00038 -25
3 OBS_003_So... 0.00270 0.00224 -0.00046 -17
4 OBS_004_So... 0.00760 0.00719 -0.00041 -5.4
5 OBS_005_So... 0.0030 -15
6 OBS_006_So 0.0207 -14
->PPM
Obsidian.devm:4
Concentrations Influence Fixed alphas
Name Z Min Max Emp
Rb 37 0.0 0.0 0.000 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Computed 0.00012
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
0.00012
Computed Fixed
Main coefficients:
Slope: 0.00001 %/Cps Offset -0.0059 Cps Quadratic 0
Computed Fixed Computed Fixed Computed Fixed
Y
Calibration Toolbox
Offset
Off On
Quadratic
Off On
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Compton
Obsidian.... Grap. Dis. Standards Alphas Intern. Std. Line Over.
For Help, press F1
Status
10:58 AM
5/1/18

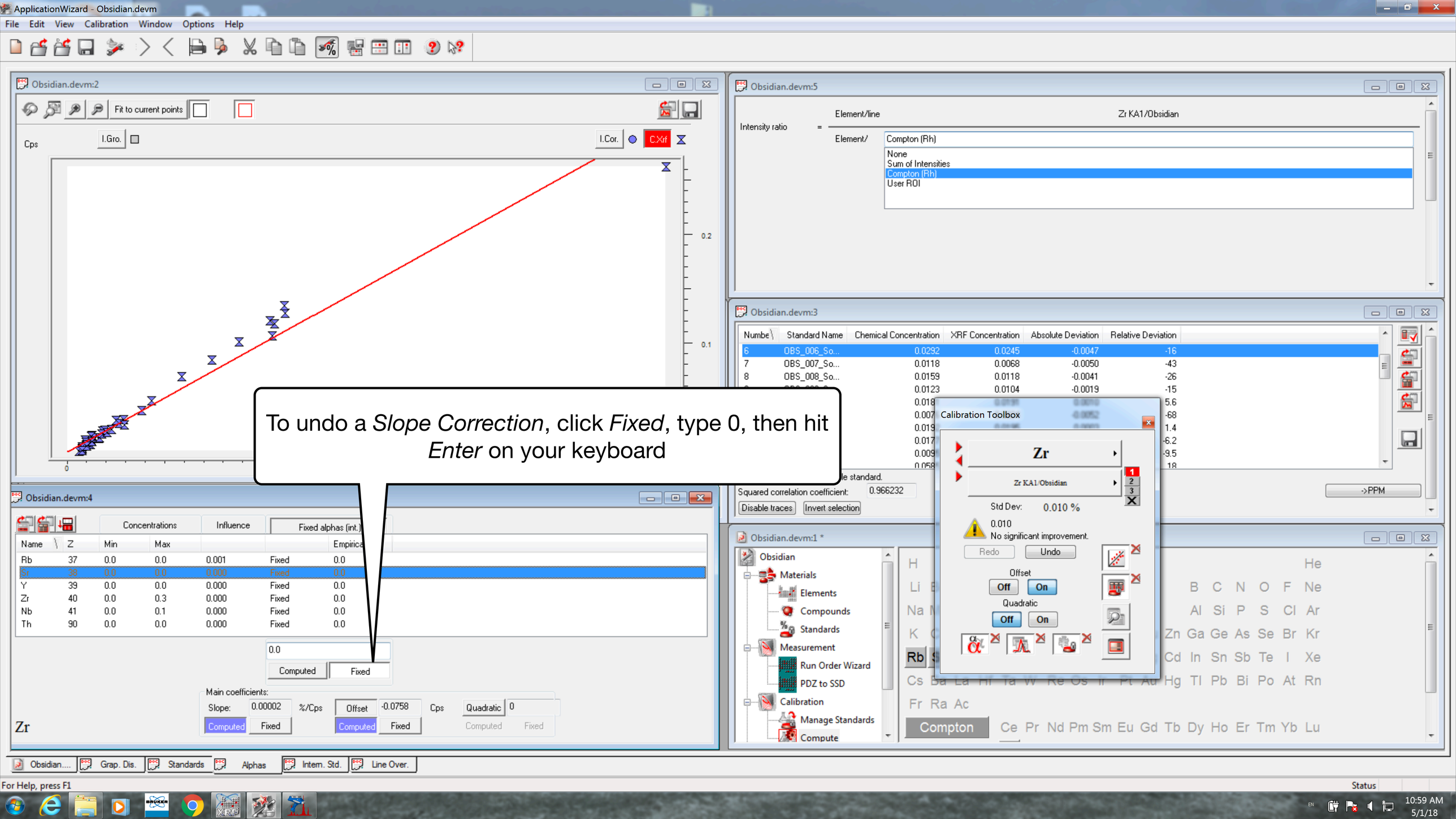

When the points are removed, they will be transparent, indicating that they are no longer used for the calibration
Click on the red forward > button and move to the next element

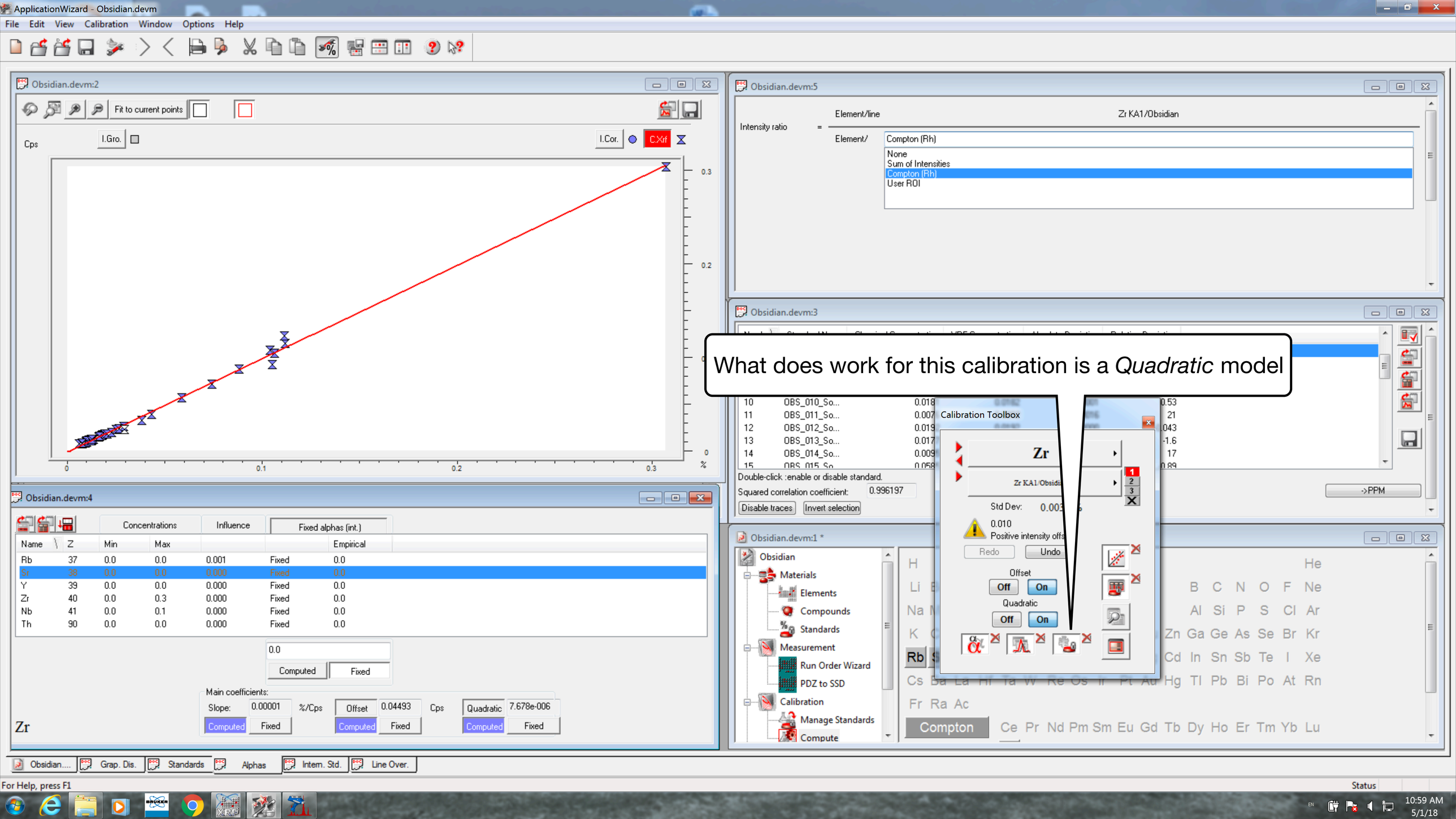

ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
Obsidian.devm:5
Element/line
Zr KA1/Obsidian
Intensity ratio
Element/
Compton (Rh)
None
Sum of Intensities
Compton (Rh)
User ROI
Obsidian.devm:3
Numbe
Standard Name
Chemical Concentration
XRF Concentration
Absolute Deviation
Relative Deviation
6 OBS_006_So... 0.0292 0.0250 -0.0042 -14
7 OBS_007_So... 0.0118 0.0073 -0.0045 -38
0.0159 0.0124 -0.0035 -22
0.0123 0.0104 -0.0019 -16
14 OBS_014_St
15 OBS_015_So
Double-click :enable or disable s
Squared correlation coefficient:
Disable traces
Invert selection
->PPM
Zirconium has a overlap with Strontium - this requires a *Line Overlap* correction
Calibration Toolbox
Zr
Zr KA1/Obsidian
Std Dev: 0.010 %
0.011
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian.devm:4
Concentrations
Influence
Fixed alphas (int.)
Name \ Z Min Max Empirical
Rb 37 0.0 0.0 0.001 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Fixed 0.0
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
0.0
Computed
Fixed
Main coefficients:
Slope: 0.00002 %/Cps
Offset -0.0688 Cps
Quadratic 0
Computed Fixed Computed Fixed Computed Fixed
Zr
Obsidian.devm:1 *
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Compton
Obsidian.... Grap. Dis. Standards Alphas Intern. Std. Line Over.
For Help, press F1
Status
10:58 AM
5/1/18

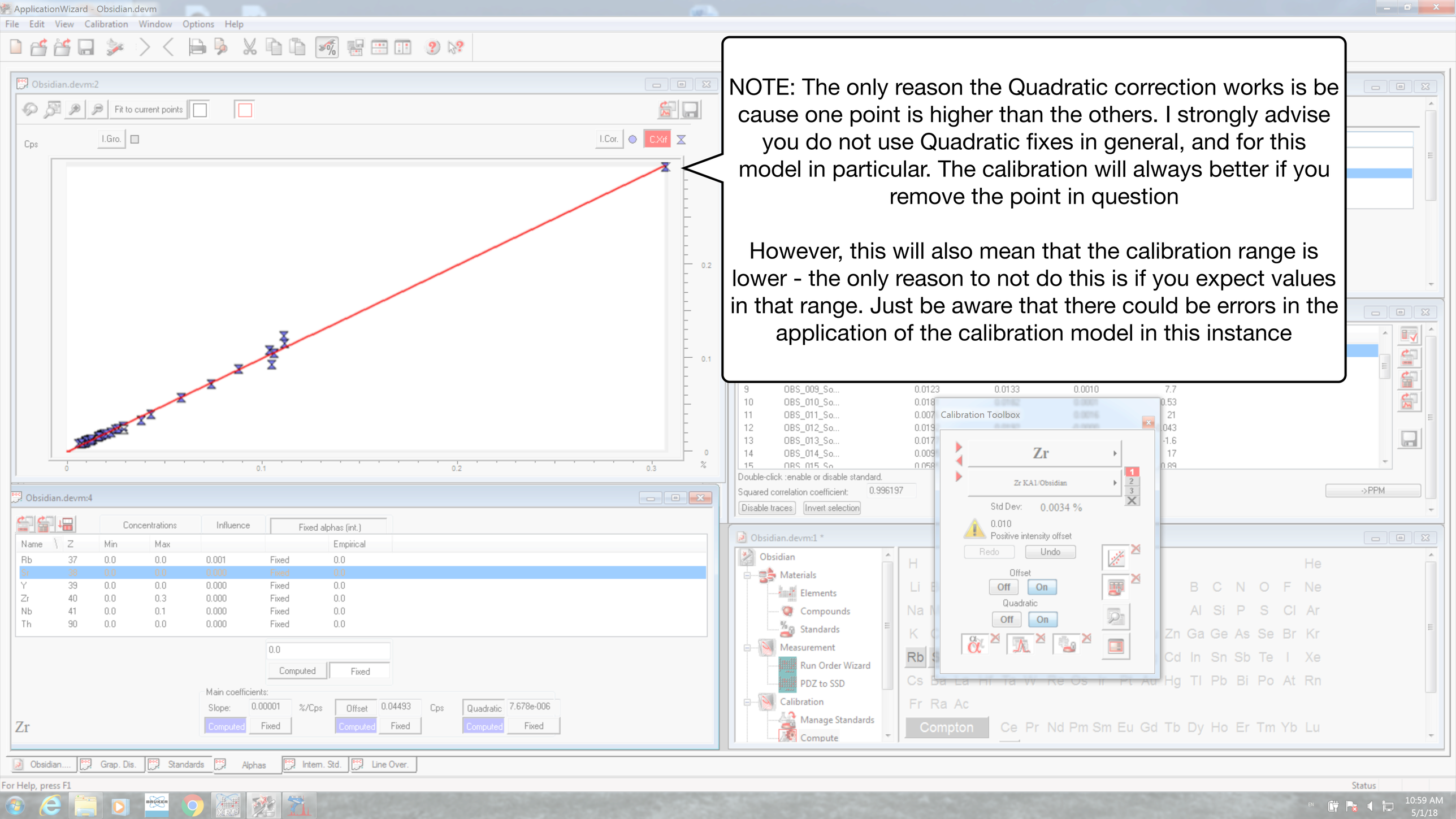

With the *Line Overlap Window* open, right click and select *Insert New*. Then choose the Strontium line which needs to be corrected for
ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
C.Xrf
Obsidian.devm:5
Obsidian.devm:6
Overlap correction for Zr KA1/Obsidian (15.776 keV)
Overlapping line:
Correct by
Measured
Factor
Search parameters
Min concentration
Distance (eV)
OK
Cancel
Th LB2,15 (15.588 keV, 26%)
Sr KB1 (15.835 keV, 16%)
Sr KB3 (15.825 keV, 8%)
Th LB1 (16.202 keV, 58%)
Th LB4 (15.642 keV, 4%)
Sr KB2 (16.083 keV, 3%)
Th LB5 (16.207 keV, 5%)
Sr KB5 (15.969 keV, 0%)
Nb KA2 (16.521 keV, 52%)
Rb KB2 (15.184 keV, 2%)
Y KA1 (14.959 keV, 100%)
Th LB3 (16.426 keV, 3%)
Nb KA1 (16.616 keV, 100%)
Rb KB1 (14.961 keV, 16%)
Nb KA3 (16.288 keV, 0%)
Y KA2 (14.882 keV, 52%)
Rb KB3 (14.951 keV, 8%)
Th LB6 (14.970 keV, 2%)
Rb KB5 (15.087 keV, 0%)
Y KB1 (16.739 keV, 16%)
Y KB3 (16.727 keV, 8%)
Overlap Energy Delta En. Remark Type Base for calculation
RF Concentration Absolute Deviation Relative Deviation
0.0250 -0.0042 -14
0.0073 -0.0045 -38
0.0124 -0.0035 -22
0.0104 -0.0019 -16
3.8
-64
1.3
-6.0
-15
18
Zr
Zr KA1/Obsidian
Std Dev: 0.010 %
0.011
Redo
Undo
Offset
Off
On
Quadratic
Off
On
->PPM
Concentrations
Influence
Fixed alphas (int.)
Name Z Min Max Empirical
Rb 37 0.0 0.0 0.001 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Fixed 0.0
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
0.0
Computed
Fixed
Main coefficients:
Slope: 0.00002 %/Cps
Offset -0.0688 Cps
Quadratic 0
Computed Fixed Computed Fixed Computed Fixed
Zr
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Compton
Obsidian.... Grap. Dis. Standards Alphas Intern. Std. Line Over.
For Help, press F1
Status
10:58 AM
5/1/18

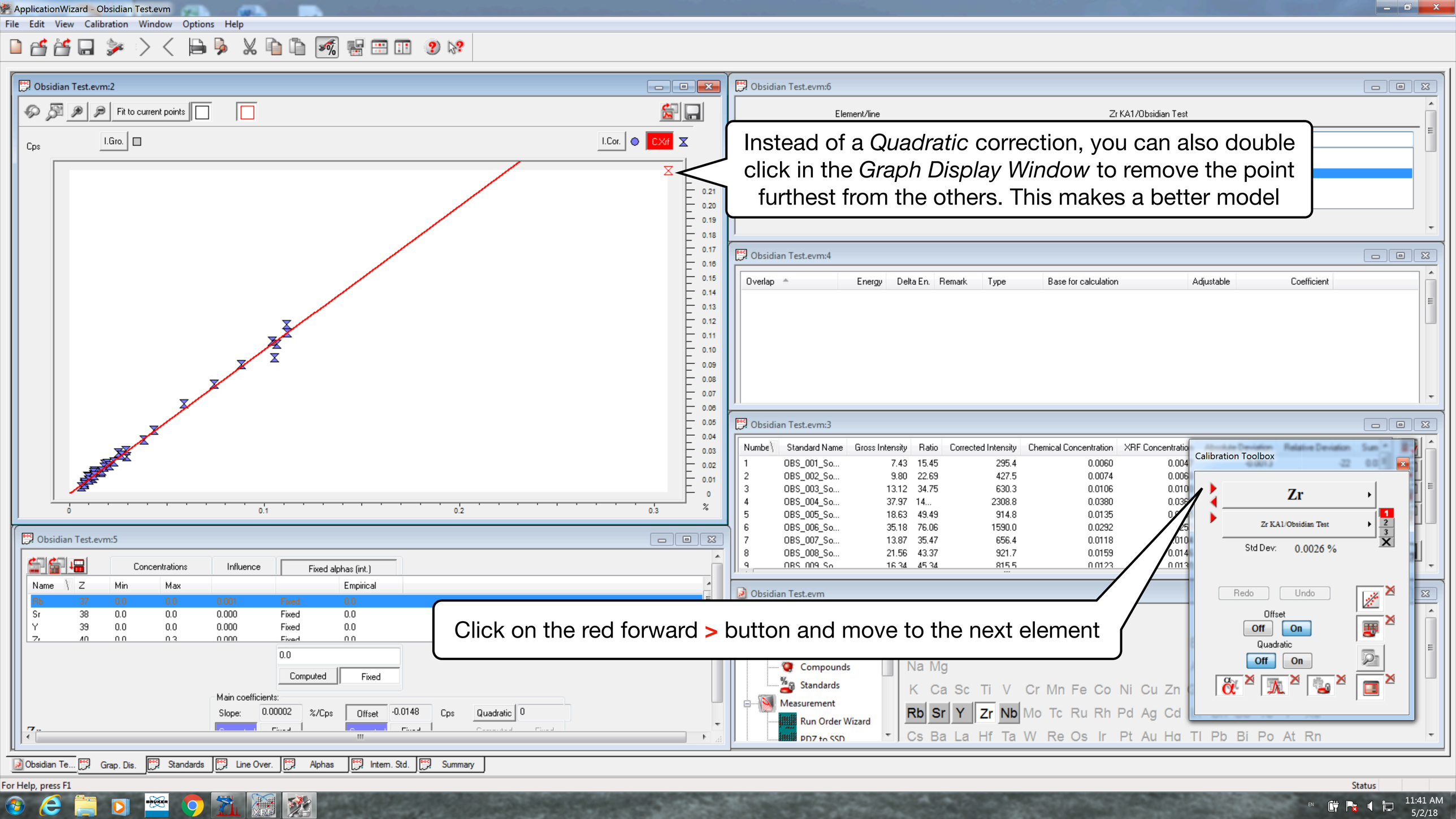

With the *Line Overlap Window* open, right click and select *Insert New*. Then choose the Strontium line which needs to be corrected for

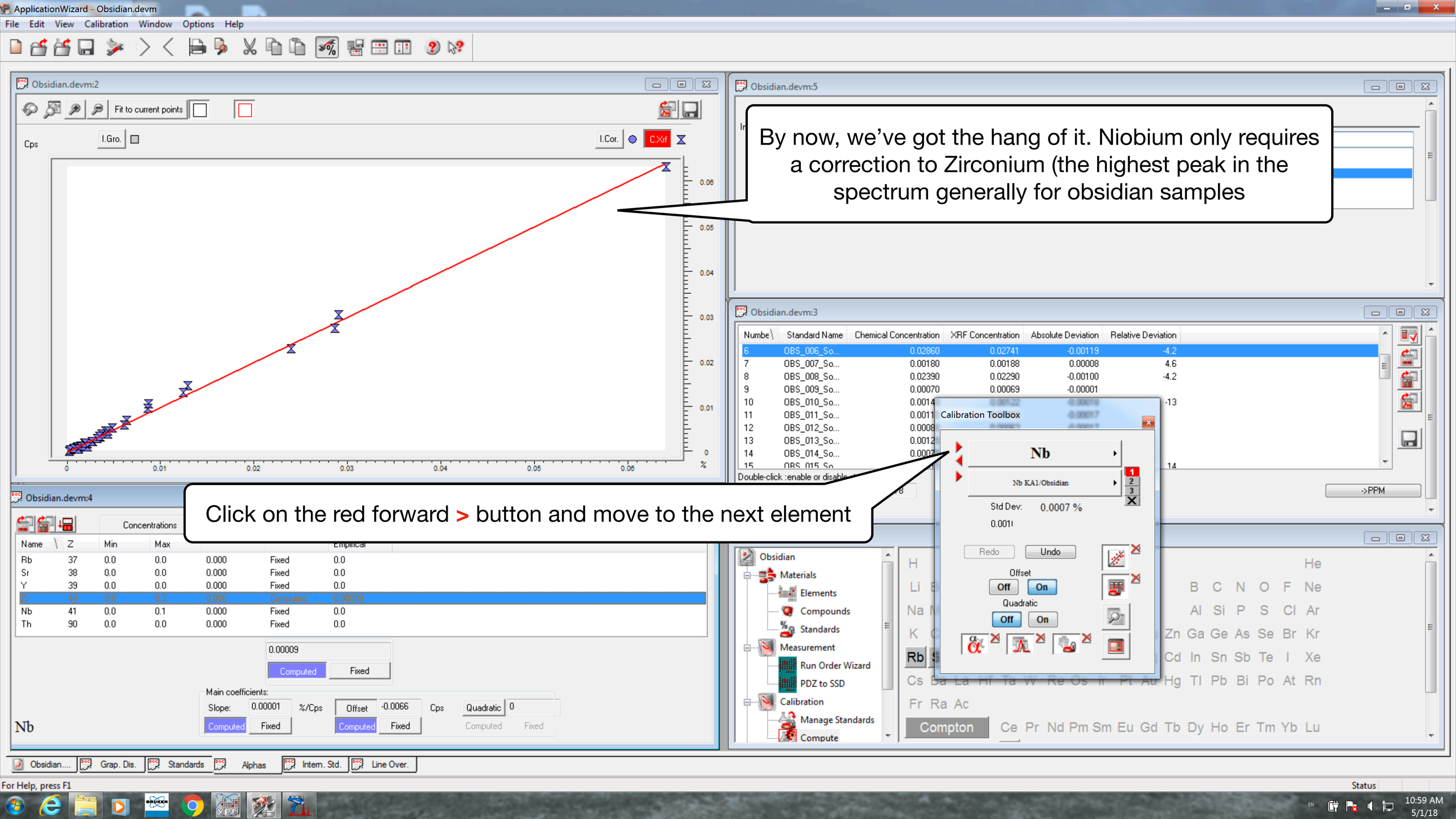

ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
Obsidian.devm:5
Element/line
Zr KA1/Obsidian
Intensity ratio
Element/
Compton (Rh)
None
Sum of Intensities
This element's calibration requires more work - this is an instance where slope corrections would be helpful. Click on the *Alphas* button
This helps, but the calibration line still needs attention. Unfortunately, a *Slope Correction* doesn't help
Absolute Deviation
Relative Deviation
-0.0047 -16
-0.0049 -42
-0.0040 -25
-0.0020 -16
10 OBS_010_So... 0.018
11 OBS_011_So... 0.007
12 OBS_012_So... 0.019
13 OBS_013_So... 0.017
14 OBS_014_So... 0.009
Double-click :enable or disable standard.
Squared correlation coefficient: 0.966362
Disable traces
Invert selection
->PPM
Calibration Tool
Zr
KA1/Obsidian
Std D: 0.010 %
No significant improvement.
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian.devm:4
Concentrations
Influence
Fixed alphas (int.)
Name Z Min Max Empirical
Rb 37 0.0 0.0 0.001 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.00078
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Fixed 0.0
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
0.00078
Computed
Fixed
Main coefficients:
Slope: 0.00002 %/Cps
Offset -0.0726 Cps
Quadratic 0
Computed Fixed Computed Fixed Computed Fixed
Zr
Obsidian.devm:1 *
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Compton
Obsidian.... Grap. Dis. Standards Alphas Intern. Std. Line Over.
For Help, press F1
Status
10:59 AM
5/1/18

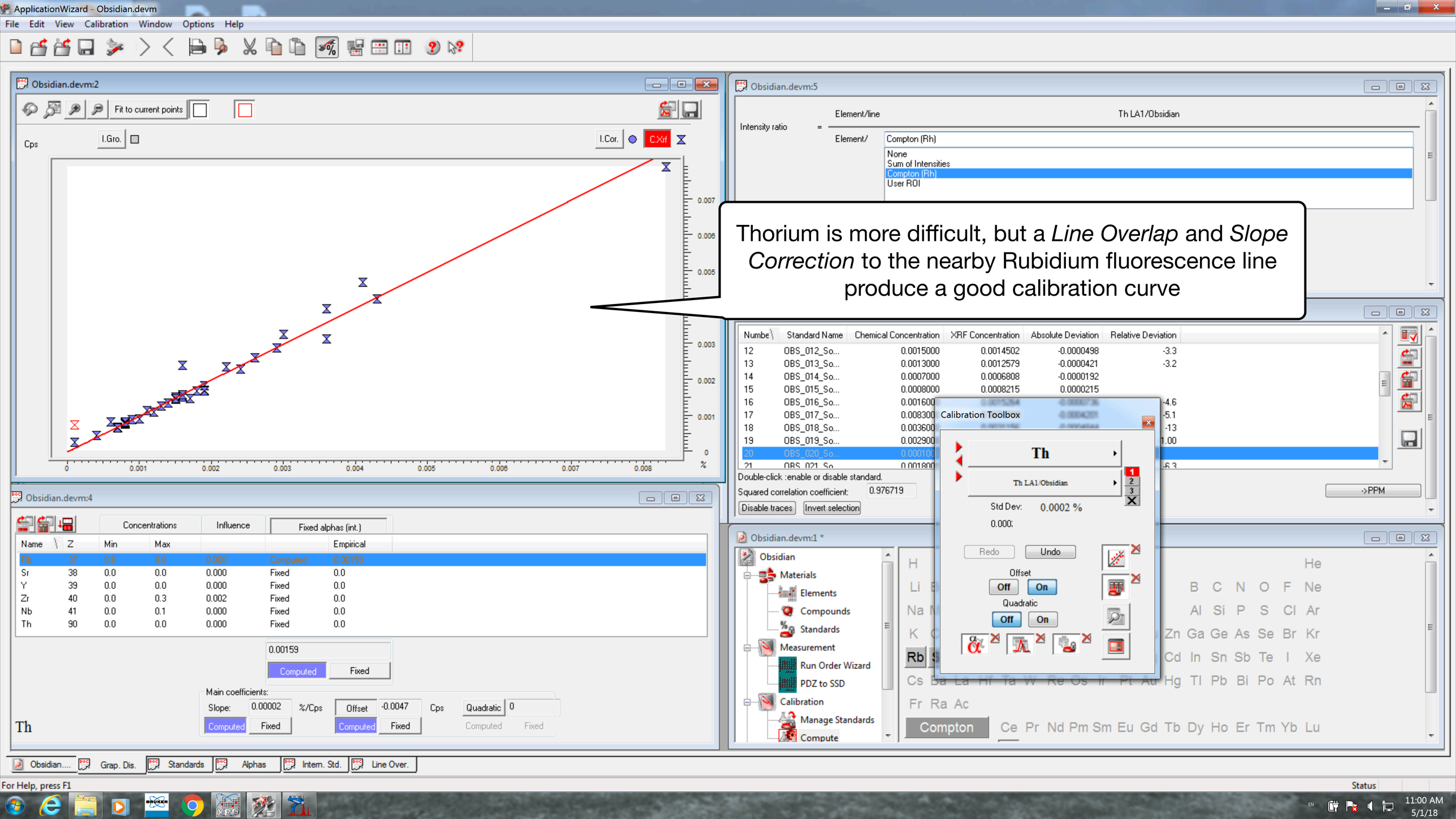

ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
0.2
0.1
0
Obsidian.devm:5
Element/line
Zr KA1/Obsidian
Intensity ratio =
Element/
Compton (Rh)
None
Sum of Intensities
Compton (Rh)
User ROI
Obsidian.devm:3
Numbe\
Standard Name
Chemical Concentration
XRF Concentration
Absolute Deviation
Relative Deviation
6 OBS_006_So... 0.0292 0.0245 -0.0047 -16
7 OBS_007_So... 0.0118 0.0068 -0.0050 -43
8 OBS_008_So... 0.0159 0.0118 -0.0041 -26
0.0123 0.0104 -0.0019 -15
Squared correlation coefficient: 0.966232
Disable traces
Invert selection
->PPM
To undo a Slope Correction, click Fixed, type 0, then hit Enter on your keyboard
Calibration Toolbox
Zr
Zr KA1/Obsidian
Std Dev: 0.010 %
0.010
No significant improvement.
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian.devm:4
Concentrations
Influence
Fixed alphas (int.)
Name \ Z Min Max Empirica
Rb 37 0.0 0.0 0.001 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Fixed 0.0
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
0.0
Computed
Fixed
Main coefficients:
Slope: 0.00002 %/Cps
Offset -0.0758 Cps
Quadratic 0
Computed Fixed Computed Fixed Computed Fixed
Zr
Obsidian.devm:1 *
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Compton
Obsidian.... Grap. Dis. Standards Alphas Intern. Std. Line Over.
For Help, press F1
Status
10:59 AM
5/1/18

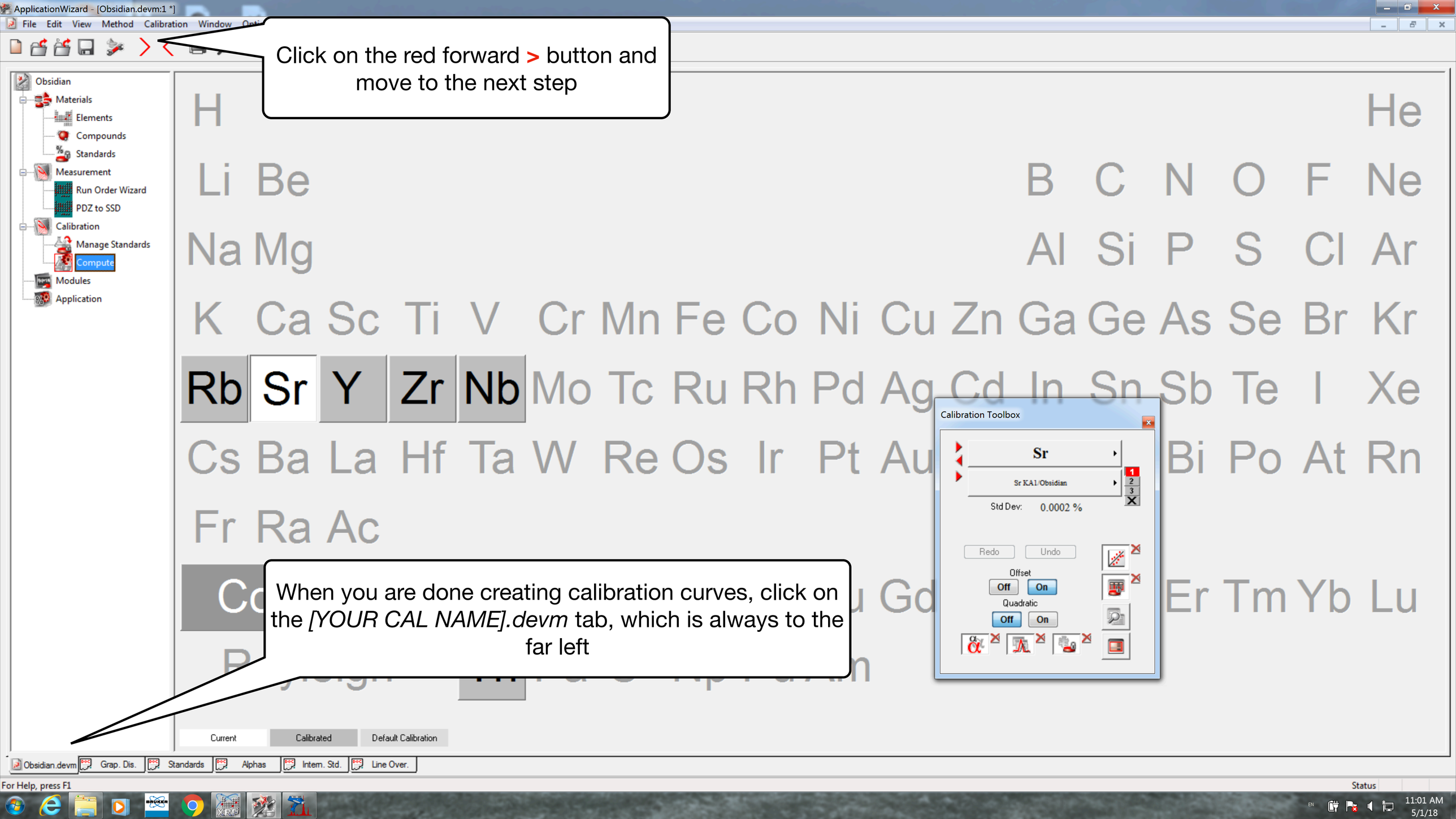

ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
Obsidian.devm:5
Element/line
Zr KA1/Obsidian
Intensity ratio
Element/
Compton (Rh)
None
Sum of Intensities
Compton (Rh)
User ROI
Obsidian.devm:3
What does work for this calibration is a Quadratic model
Double-click :enable or disable standard.
Squared correlation coefficient:
0.996197
Disable traces
Invert selection
->PPM
Calibration Toolbox
Zr
Std Dev:
0.010
Positive intensity offs
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian.devm:4
Concentrations
Influence
Fixed alphas (int.)
Name Z Min Max Empirical
Rb 37 0.0 0.0 0.001 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Fixed 0.0
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
Computed
Fixed
Main coefficients:
Slope: 0.00001 %/Cps
Offset 0.04493 Cps
Quadratic 7.678e-006
Zr
Obsidian.devm:1 *
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Compton
Obsidian.... Grap. Dis. Standards Alphas Intern. Std. Line Over.
For Help, press F1
Status
10:59 AM
5/1/18


NOTE: The only reason the Quadratic correction works is be cause one point is higher than the others. I strongly advise you do not use Quadratic fixes in general, and for this model in particular. The calibration will always better if you remove the point in question
However, this will also mean that the calibration range is lower - the only reason to not do this is if you expect values in that range. Just be aware that there could be errors in the application of the calibration model in this instance
ApplicationWizard - Obsidian.devm
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
C.Xrf
Obsidian.devm:4
Concentrations
Influence
Fixed alphas (int.)
Name
Z
Min
Max
Empirical
Rb 37 0.0 0.0 0.001 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Fixed 0.0
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
Computed
Fixed
Main coefficients:
Slope: 0.00001 %/Cps
Offset 0.04493 Cps
Quadratic 7.678e-006
Zr
Calibration Toolbox
Zr KA1/Obsidian
Std Dev: 0.0034 %
0.010
Positive intensity offset
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Double-click :enable or disable standard.
Squared correlation coefficient: 0.996197
Disable traces
Invert selection
->PPM
Obsidian.devm:1 *
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Compton
Obsidian....
Grap. Dis.
Standards
Alphas
Intern. Std.
Line Over.
For Help, press F1
Status
10:59 AM
5/1/18

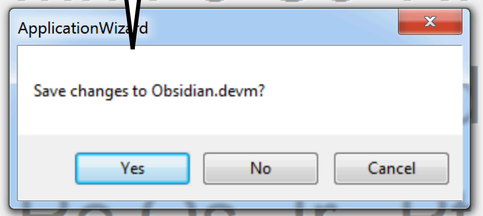

ApplicationWizard - Obsidian Test.evm
File Edit View Calibration Window Options Help
Obsidian Test.evm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
Obsidian Test.evm:6
Element/line
Zr KA1/Obsidian Test
Instead of a Quadratic correction, you can also double click in the Graph Display Window to remove the point furthest from the others. This makes a better model
Obsidian Test.evm:4
Overlap
Energy
Delta En.
Remark
Type
Base for calculation
Adjustable
Coefficient
Obsidian Test.evm:3
Numbe
Standard Name
Gross Intensity
Ratio
Corrected Intensity
Chemical Concentration
XRF Concentratio
1 OBS_001_So... 7.43 15.45 295.4 0.0060
2 OBS_002_So... 9.80 22.69 427.5 0.0074
3 OBS_003_So... 13.12 34.75 630.3 0.0106
4 OBS_004_So... 37.97 14... 2308.8 0.0380
5 OBS_005_So... 18.63 49.49 914.8 0.0135
6 OBS_006_So... 35.18 76.06 1590.0 0.0292
7 OBS_007_So... 13.87 35.47 656.4 0.0118
8 OBS_008_So... 21.56 43.37 921.7 0.0159
Calibration Toolbox
Zr
Zr KA1/Obsidian Test
Std Dev: 0.0026 %
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian Test.evm:5
Concentrations
Influence
Fixed alphas (int.)
Name Z Min Max Empirical
Rb 37 0.0 0.0 0.001 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
0.0
Computed
Fixed
Main coefficients:
Slope: 0.00002 %/Cps
Offset -0.0148 Cps
Quadratic 0
Obsidian Test.evm
Compounds
Standards
Measurement
Run Order Wizard
Na Mg
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd
Cs Ba La Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Click on the red forward > button and move to the next element
Obsidian Te...
Grap. Dis.
Standards
Line Over.
Alphas
Intern. Std.
Summary
For Help, press F1
Status
11:41 AM
5/2/18

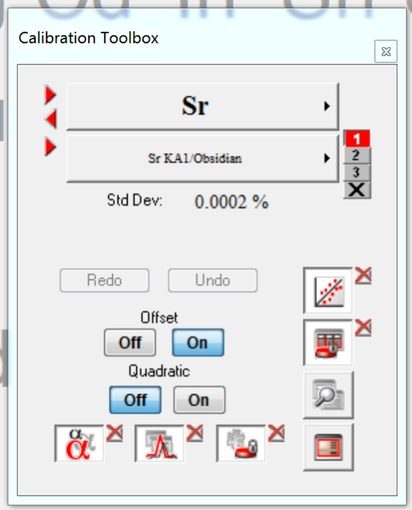

ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
C.Xrf
By now, we've got the hang of it. Niobium only requires a correction to Zirconium (the highest peak in the spectrum generally for obsidian samples
Obsidian.devm:5
Obsidian.devm:3
Numbe
Standard Name
Chemical Concentration
XRF Concentration
Absolute Deviation
Relative Deviation
Double-click :enable or disable
->PPM
Calibration Toolbox
Nb
Nb KA1/Obsidian
Std Dev: 0.0007 %
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Click on the red forward > button and move to the next element
Obsidian.devm:4
Concentrations
Name
Z
Min
Max
Empirical
Rb 37 0.0 0.0 0.000 Fixed 0.0
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.000 Computed 0.00009
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
0.00009
Computed
Fixed
Main coefficients:
Slope:
0.00001
%/Cps
Offset
-0.0066
Cps
Quadratic
0
Computed
Fixed
Nb
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Compton
Obsidian....
Grap. Dis.
Standards
Alphas
Intern. Std.
Line Over.
For Help, press F1
Status
10:59 AM
5/1/18

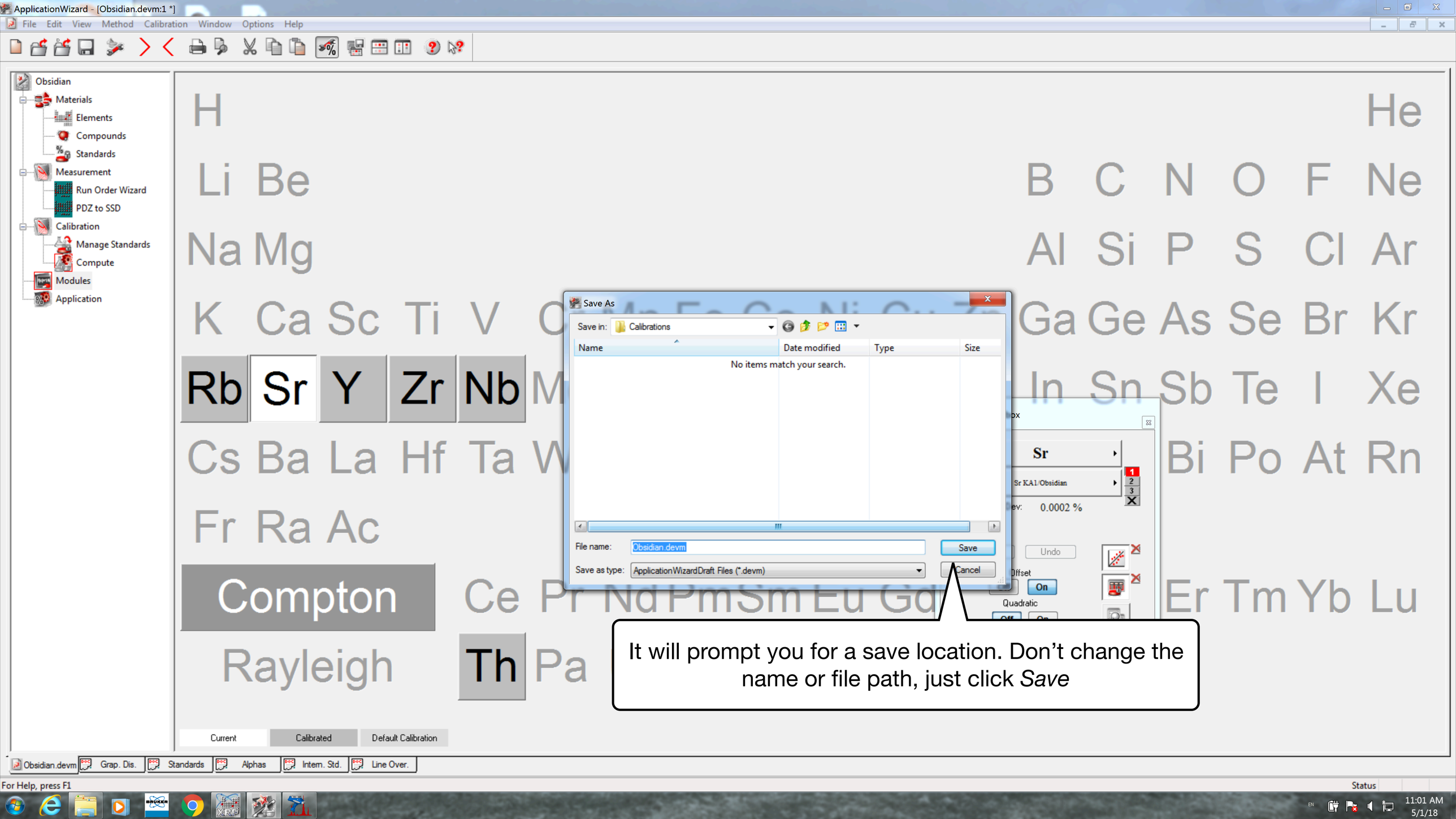

ApplicationWizard - Obsidian.devm
File Edit View Calibration Window Options Help
Obsidian.devm:2
Fit to current points
Cps
I.Gro.
I.Cor.
CXrf
Obsidian.devm:5
Element/line
Th LA1/Obsidian
Intensity ratio
Element/
Compton (Rh)
None
Sum of Intensities
Compton (Rh)
User ROI
Thorium is more difficult, but a Line Overlap and Slope Correction to the nearby Rubidium fluorescence line produce a good calibration curve
Numbe
Standard Name
Chemical Concentration
XRF Concentration
Absolute Deviation
Relative Deviation
12 OBS_012_So... 0.0015000 0.0014502 -0.0000498 -3.3
13 OBS_013_So... 0.0013000 0.0012579 -0.0000421 -3.2
14 OBS_014_So... 0.0007000 0.0006808 -0.0000192
15 OBS_015_So... 0.0008000 0.0008215 0.0000215
16 OBS_016_So... -4.6
17 OBS_017_So... -5.1
18 OBS_018_So... -13
19 OBS_019_So... 1.00
20 OBS_020_So...
21 OBS_021_So...
Double-click :enable or disable standard.
Squared correlation coefficient: 0.976719
Disable traces
Invert selection
->PPM
Calibration Toolbox
Th
Th LA1/Obsidian
Std Dev: 0.0002 %
Redo
Undo
Offset
Off
On
Quadratic
Off
On
Obsidian.devm:4
Concentrations
Influence
Fixed alphas (int.)
Name Z Min Max Empirical
Rb 37 0.0 0.0 0.000 Computed 0.00159
Sr 38 0.0 0.0 0.000 Fixed 0.0
Y 39 0.0 0.0 0.000 Fixed 0.0
Zr 40 0.0 0.3 0.002 Fixed 0.0
Nb 41 0.0 0.1 0.000 Fixed 0.0
Th 90 0.0 0.0 0.000 Fixed 0.0
0.00159
Computed
Fixed
Main coefficients:
Slope: 0.00002 %/Cps
Offset -0.0047 Cps
Quadratic 0
Th
Obsidian.devm:1 *
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Compton
Obsidian.... Grap. Dis. Standards Alphas Intern. Std. Line Over.
For Help, press F1
Status
11:00 AM
5/1/18

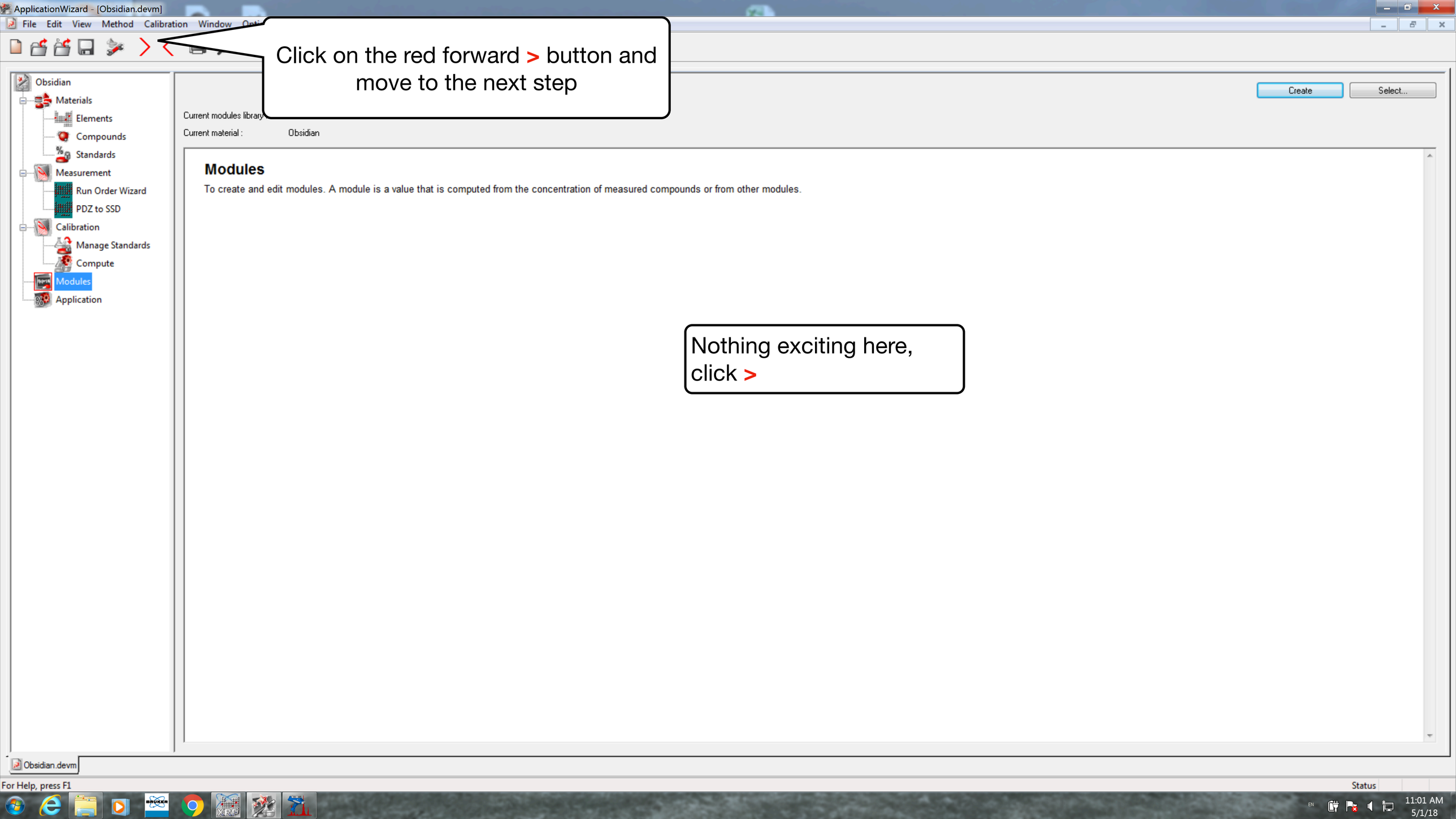

ApplicationWizard - [Obsidian.devm:1 *]
File Edit View Method Calibration Window
Click on the red forward > button and move to the next step
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Modules
Application
Rb Sr Y Zr Nb
Calibration Toolbox
Sr
Sr KA1/Obsidian
Std Dev: 0.0002 %
Redo Undo
Offset
Off On
Quadratic
Off On
When you are done creating calibration curves, click on the [YOUR CAL NAME].devm tab, which is always to the far left
Current Calibrated Default Calibration
Obsidian.devm Grap. Dis. Standards Alphas Intern. Std. Line Over.
For Help, press F1
Status
11:01 AM
5/1/18

When prompted, say yes to safe a *.devm*, or draft calibration file. This will be saved to *Your Cal/Std SSD/ Libraries/Calibrations* on your computer






ApplicationWizard - [Obsidian.devm:1 *]
File Edit View Method Calibration Window Options Help
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Modules
Application
Save As
Save in: Calibrations
Name
Date modified
Type
Size
No items match your search.
File name: Obsidian.devm
Save as type: ApplicationWizardDraft Files (*.devm)
Save
Cancel
Sr
Sr KA1/Obsidian
0.0002 %
Undo
On
Quadratic
Compton
Rayleigh
Current
Calibrated
Default Calibration
Obsidian.devm
Grap. Dis.
Standards
Alphas
Intern. Std.
Line Over.
For Help, press F1
Status
11:01 AM
5/1/18
It will prompt you for a save location. Don't change the name or file path, just click *Save*


ApplicationWizard - [Obsidian.devm]
File Edit View Method Calibration Window
Click on the red forward > button and move to the next step
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Modules
Application
Create
Select...
Current modules library
Current material : Obsidian
Modules
To create and edit modules. A module is a value that is computed from the concentration of measured compounds or from other modules.
Nothing exciting here, click >
Obsidian.devm
For Help, press F1
Status
11:01 AM
5/1/18

ApplicationWizard - [Obsidian.devm]

File Edit View Method Calibration Window Options Help

Obsidian
- Materials
  - Elements
  - Compounds
  - Standards
- Measurement
  - Run Order Wizard
  - PDZ to SSD
- Calibration
  - Manage Standards
  - Compute
- Modules
- Application

Create

Current material : Obsidian

Current preparation : Solids

Application

Purpose

Creation of the evaluation model (EVM file) associated to the material.

Overview

The evaluation model has two roles. The first one is to link the different files of a method (FCL, MM, WZM, MLB,

The second one is to define hypotheses on the unknown sample: matrix (i.e. compound not measured but estim
measured but is considered to be the same amongst all samples), normalization etc.

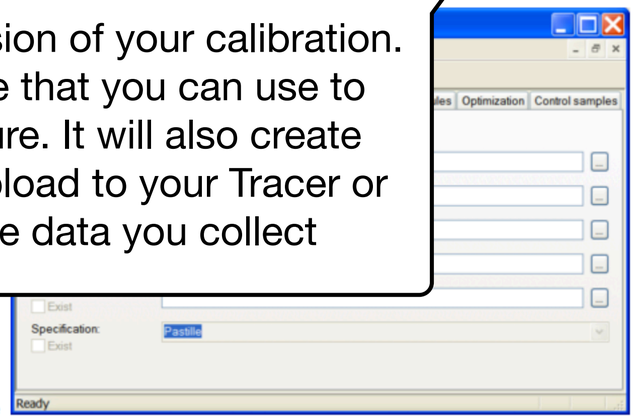
How?

The maintenance of evaluation models is made by an external program called ApplicationSetup.

If the default evaluation model for the current material does not already exist, click on **Create** and it will be automatically created. To view or modify the default model, click on **Edit** and ApplicationWizard will open ApplicationSetup for you.

Note

The matrix (100%-sum of the other compounds) can be set at the **Material** level (select **Column Balance** for the compound at the **Standard Materials** step). This works when the standards have the same matrix as the unknown; if it is not the case (e.g. the standards are dry but the unknowns are hydrated), define the matrix in the evaluation model.



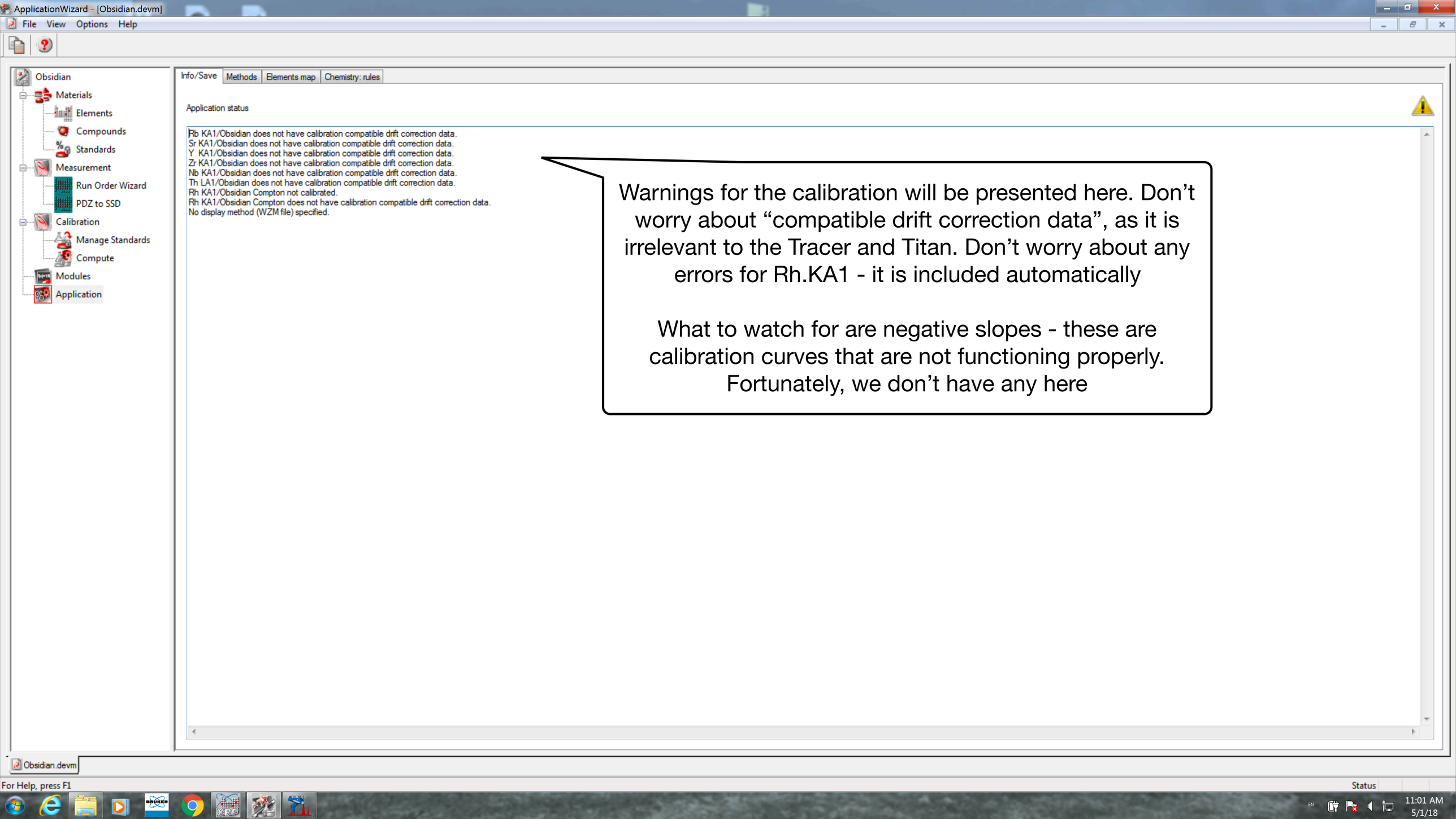
It is now time to save the final version of your calibration. This will both create the *.evm* file that you can use to modify the calibration in the future. It will also create the *.appinstall* file that you can upload to your Tracer or Titan to automatically calibrate data you collect

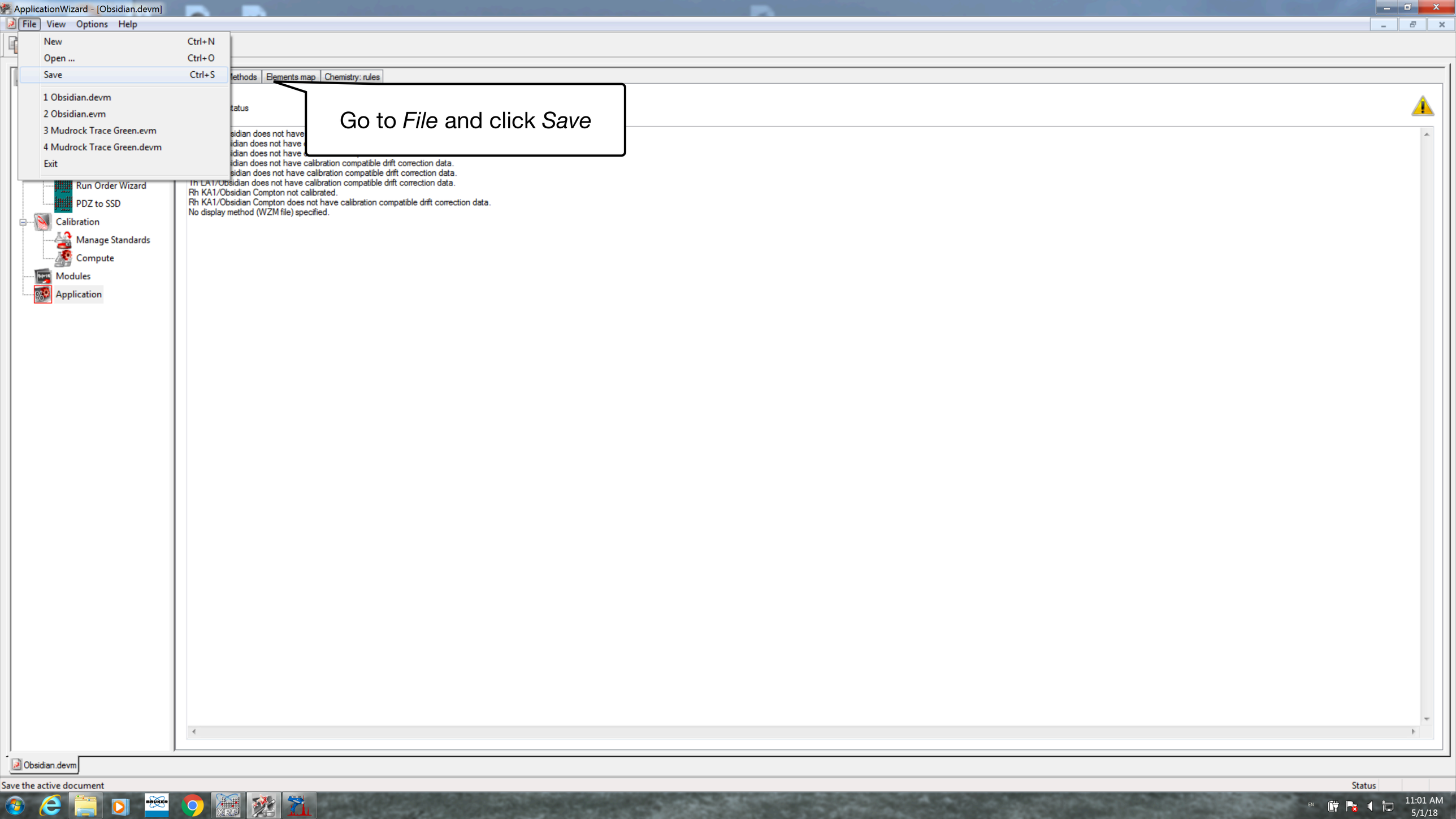
Obsidian.devm

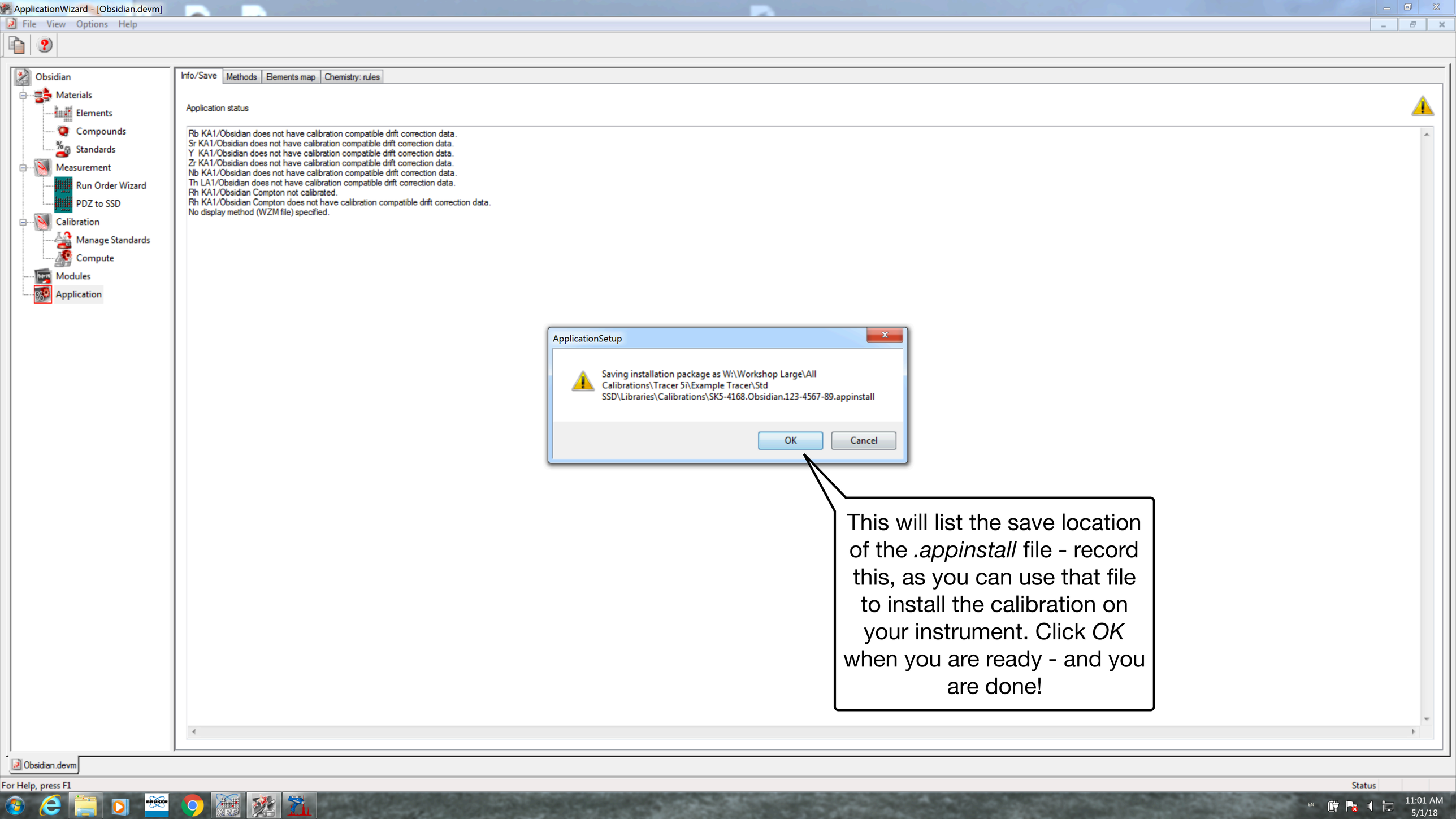
For Help, press F1

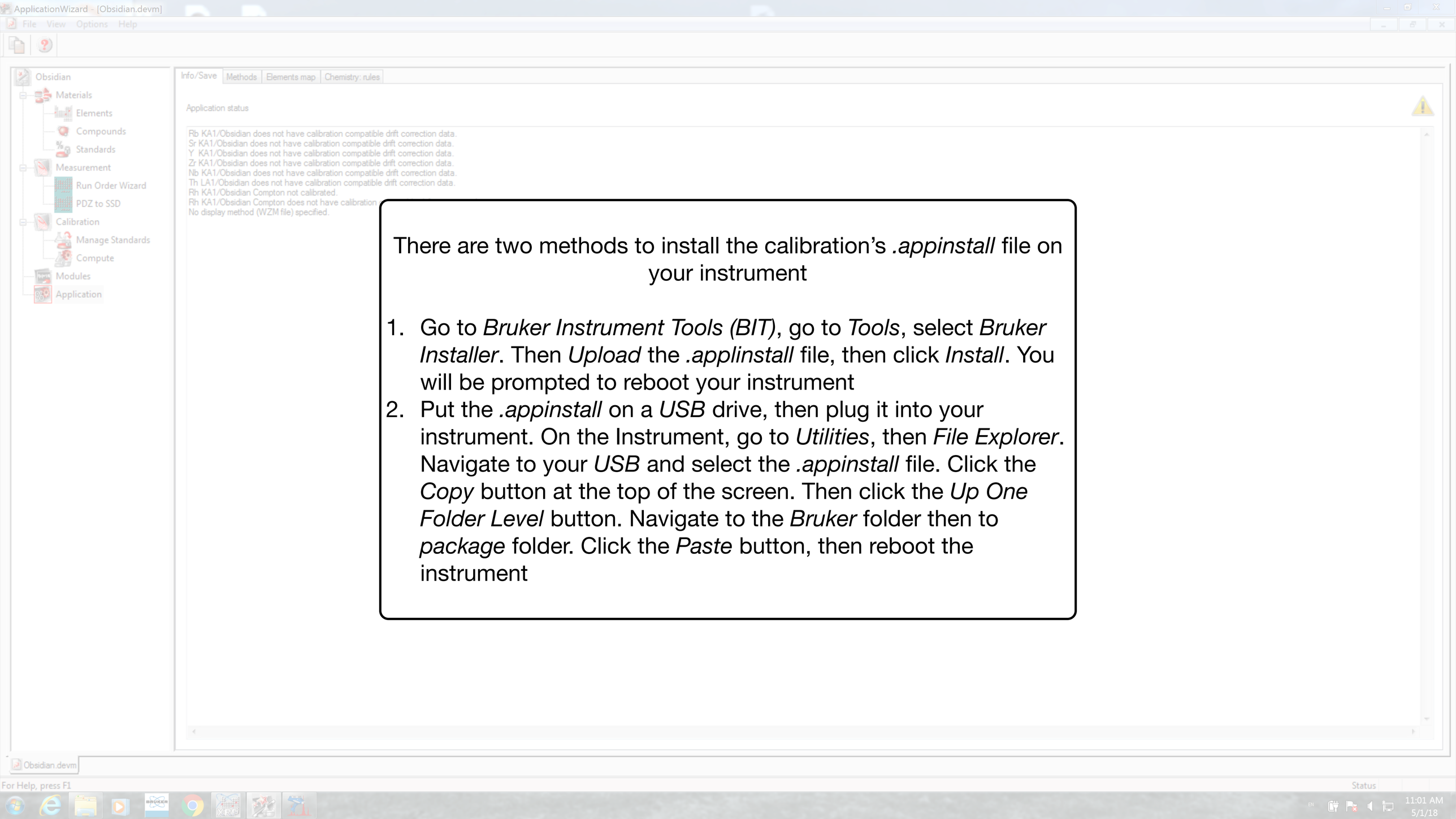
Status

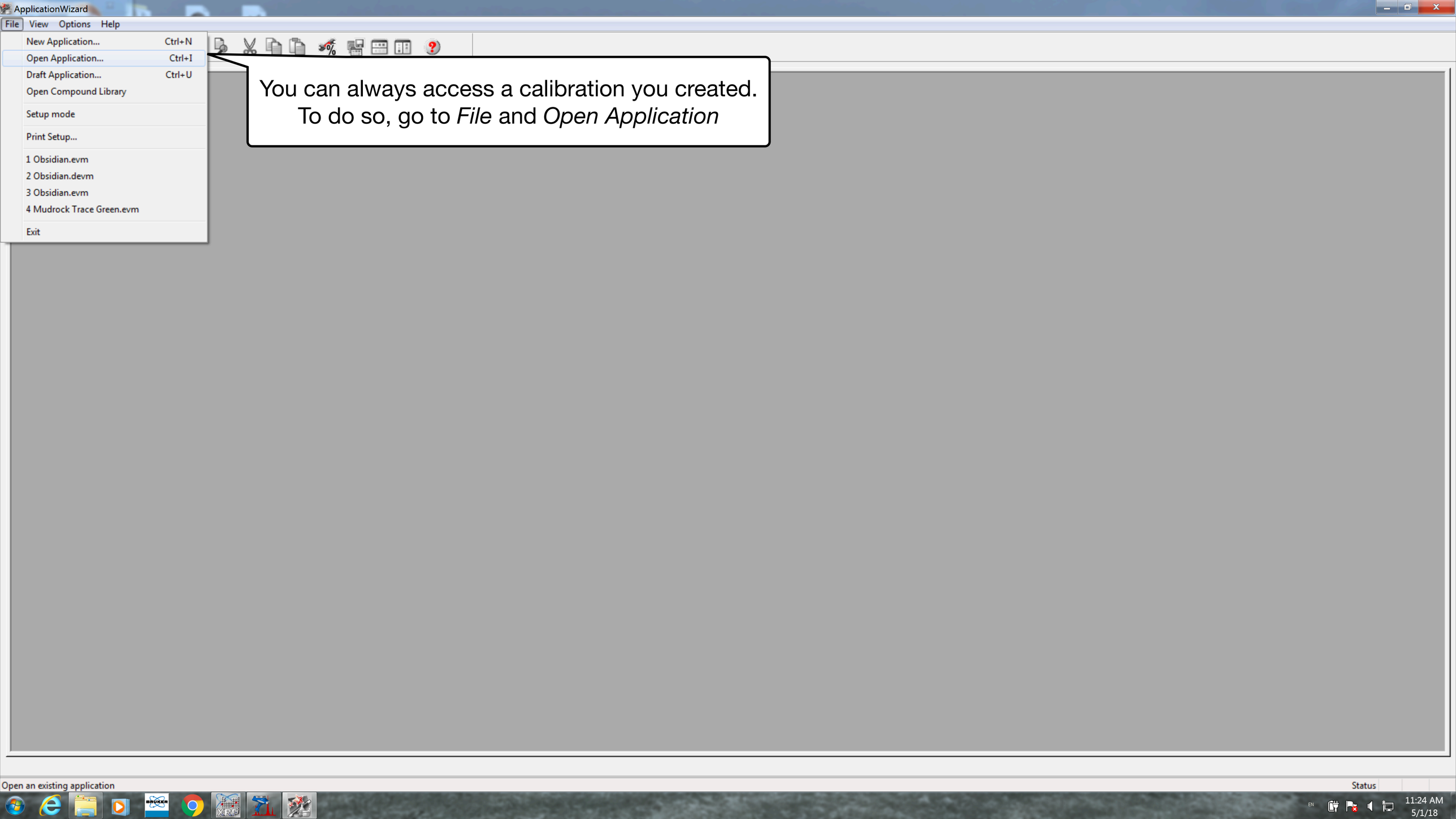
11:01 AM
5/1/18

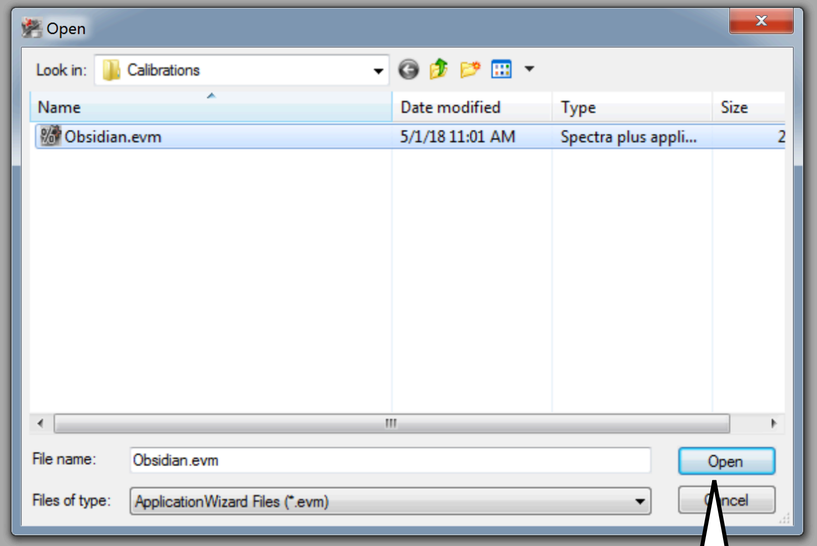

ApplicationWizard - [Obsidian.devm]
File View Options Help
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Modules
Application
Info/Save
Methods
Elements map
Chemistry: rules
Application status
Rb KA1/Obsidian does not have calibration compatible drift correction data.
Sr KA1/Obsidian does not have calibration compatible drift correction data.
Y KA1/Obsidian does not have calibration compatible drift correction data.
Zr KA1/Obsidian does not have calibration compatible drift correction data.
Nb KA1/Obsidian does not have calibration compatible drift correction data.
Th LA1/Obsidian does not have calibration compatible drift correction data.
Rh KA1/Obsidian Compton not calibrated.
Rh KA1/Obsidian Compton does not have calibration compatible drift correction data.
No display method (WZM file) specified.
Warnings for the calibration will be presented here. Don't worry about "compatible drift correction data", as it is irrelevant to the Tracer and Titan. Don't worry about any errors for Rh.KA1 - it is included automatically
What to watch for are negative slopes - these are calibration curves that are not functioning properly. Fortunately, we don't have any here
Obsidian.devm
For Help, press F1
Status
11:01 AM
5/1/18


ApplicationWizard - [Obsidian.devm]
File
View
Options
Help
New Ctrl+N
Open ... Ctrl+O
Save Ctrl+S
1 Obsidian.devm
2 Obsidian.evm
3 Mudrock Trace Green.evm
4 Mudrock Trace Green.devm
Exit
Go to *File* and click *Save*
Elements map
Chemistry: rules
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Modules
Application
Rh KA1/Obsidian Compton not calibrated.
Rh KA1/Obsidian Compton does not have calibration compatible drift correction data.
No display method (WZM file) specified.
Obsidian.devm
Save the active document
Status
11:01 AM
5/1/18


ApplicationWizard - [Obsidian.devm]
File View Options Help
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Modules
Application
Info/Save
Methods
Elements map
Chemistry: rules
Application status
Rb KA1/Obsidian does not have calibration compatible drift correction data.
Sr KA1/Obsidian does not have calibration compatible drift correction data.
Y KA1/Obsidian does not have calibration compatible drift correction data.
Zr KA1/Obsidian does not have calibration compatible drift correction data.
Nb KA1/Obsidian does not have calibration compatible drift correction data.
Th LA1/Obsidian does not have calibration compatible drift correction data.
Rh KA1/Obsidian Compton not calibrated.
Rh KA1/Obsidian Compton does not have calibration compatible drift correction data.
No display method (WZM file) specified.
ApplicationSetup
Saving installation package as W:\Workshop Large\All Calibrations\Tracer 5i\Example Tracer\Std SSD\Libraries\Calibrations\SK5-4168.Obsidian.123-4567-89.appinstall
OK
Cancel
This will list the save location of the .appinstall file - record this, as you can use that file to install the calibration on your instrument. Click OK when you are ready - and you are done!
Obsidian.devm
For Help, press F1
Status
11:01 AM
5/1/18


There are two methods to install the calibration's .appinstall file on your instrument
1. Go to Bruker Instrument Tools (BIT), go to Tools, select Bruker Installer. Then Upload the .applinstall file, then click Install. You will be prompted to reboot your instrument
2. Put the .appinstall on a USB drive, then plug it into your instrument. On the Instrument, go to Utilities, then File Explorer. Navigate to your USB and select the .appinstall file. Click the Copy button at the top of the screen. Then click the Up One Folder Level button. Navigate to the Bruker folder then to package folder. Click the Paste button, then reboot the instrument


ApplicationWizard
File
View
Options
Help
New Application... Ctrl+N
Open Application... Ctrl+I
Draft Application... Ctrl+U
Open Compound Library
Setup mode
Print Setup...
1 Obsidian.evm
2 Obsidian.devm
3 Obsidian.evm
4 Mudrock Trace Green.evm
Exit
You can always access a calibration you created.
To do so, go to *File* and *Open Application*
Open an existing application
Status
11:24 AM
5/1/18



Choose the calibration you want to open and click *OK*

ApplicationWizard - [Obsidian.evm]

File Edit View Method Calibration Window Options Help

Obsidian
- Materials
  - Elements
  - Compounds
  - Standards
- Measurement
  - Run Order Wizard
  - PDZ to SSD
- Calibration
  - Manage Standards
  - Compute
- Modules
- Application

Edit

Current material : Obsidian

Current preparation : Solids

Application

Purpose

Creation of the evaluation model (EVM file) associated to the material.

Overview

The evaluation model has two roles. The first one is to link the different files of a method (FCL, MM, WZM, MLB...) together. This is not

The second one is to define hypotheses on the unknown sample: matrix (i.e. compound not measured but estimated by balance to 10
measured but is considered to be the same amongst all samples), normalization etc.

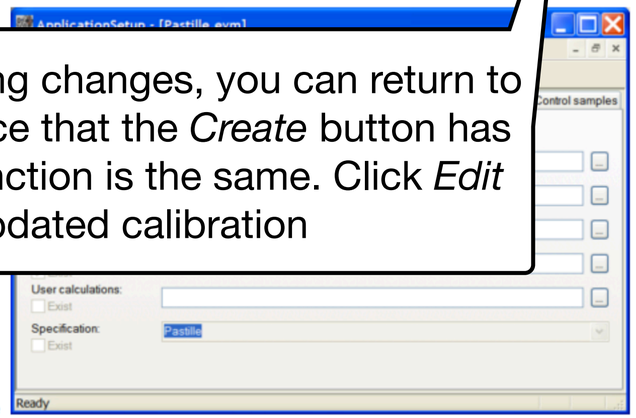
How?

The maintenance of evaluation models is made by an external program called ApplicationSetup.

If the default evaluation model for the current material does not already exist, click on **Create** and it will be automatically created. To view or modify the default model, click on **Edit** and ApplicationWizard will open ApplicationSetup for you.

Note

The matrix (100%-sum of the other compounds) can be set at the **Material** level (select **Column Balance** for the compound at the **Standard Materials** step). This works when the standards have the same matrix as the unknown; if it is not the case (e.g. the standards are dry but the unknowns are hydrated), define the matrix in the evaluation model.



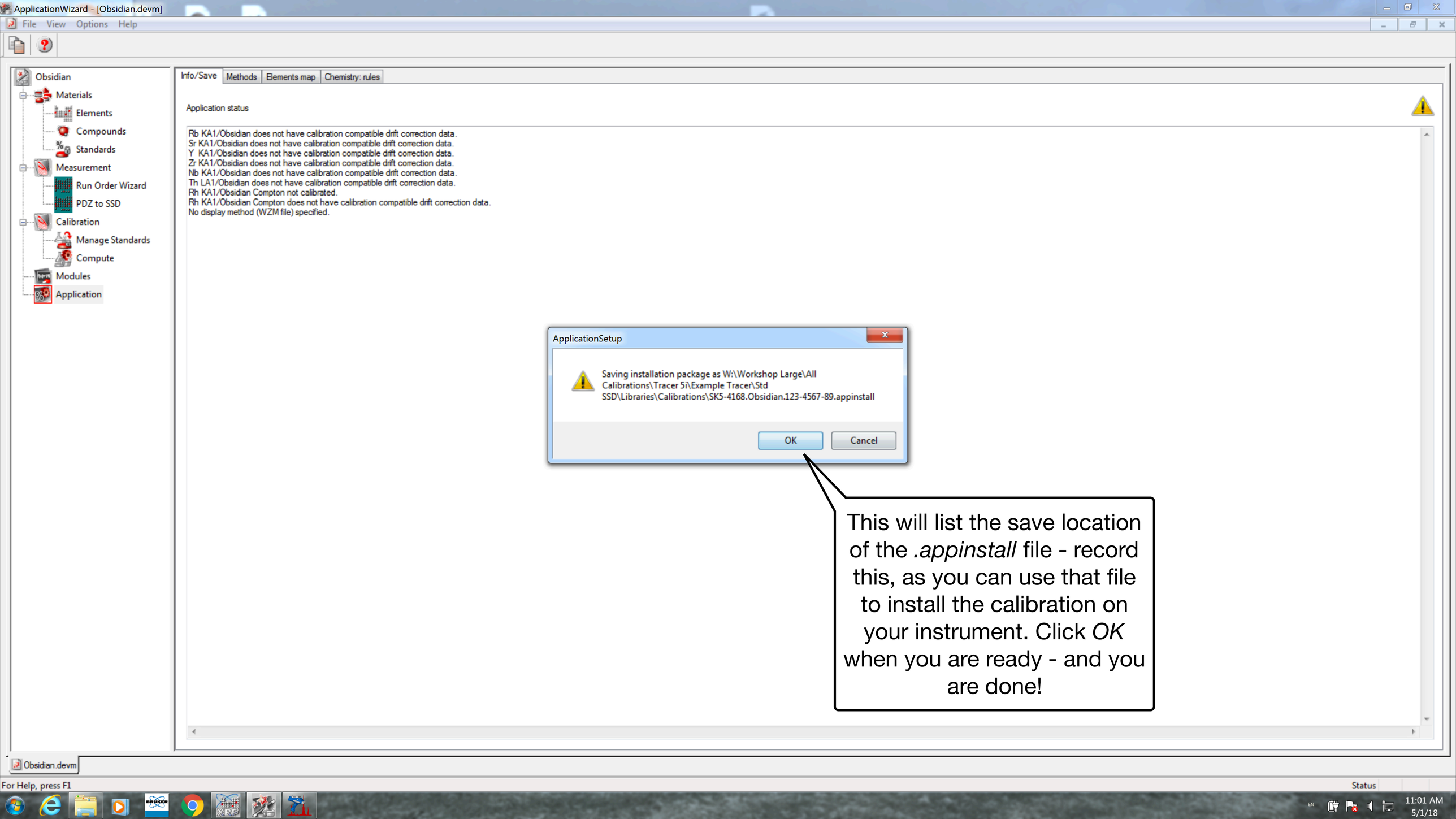
When you are done making changes, you can return to *Application*. You will notice that the *Create* button has changed to *Edit* - the function is the same. Click *Edit* to save the updated calibration

Obsidian.evm

For Help, press F1

Status

11:02 AM
5/1/18


ApplicationWizard - [Obsidian.devm]
File View Options Help
Obsidian
Materials
Elements
Compounds
Standards
Measurement
Run Order Wizard
PDZ to SSD
Calibration
Manage Standards
Compute
Modules
Application
Info/Save
Methods
Elements map
Chemistry: rules
Application status
Rb KA1/Obsidian does not have calibration compatible drift correction data.
Sr KA1/Obsidian does not have calibration compatible drift correction data.
Y KA1/Obsidian does not have calibration compatible drift correction data.
Zr KA1/Obsidian does not have calibration compatible drift correction data.
Nb KA1/Obsidian does not have calibration compatible drift correction data.
Th LA1/Obsidian does not have calibration compatible drift correction data.
Rh KA1/Obsidian Compton not calibrated.
Rh KA1/Obsidian Compton does not have calibration compatible drift correction data.
No display method (WZM file) specified.
ApplicationSetup
Saving installation package as W:\Workshop Large\All Calibrations\Tracer 5i\Example Tracer\Std SSD\Libraries\Calibrations\SK5-4168.Obsidian.123-4567-89.appinstall
OK
Cancel
This will list the save location of the .appinstall file - record this, as you can use that file to install the calibration on your instrument. Click OK when you are ready - and you are done!
Obsidian.devm
For Help, press F1
Status
11:01 AM
5/1/18