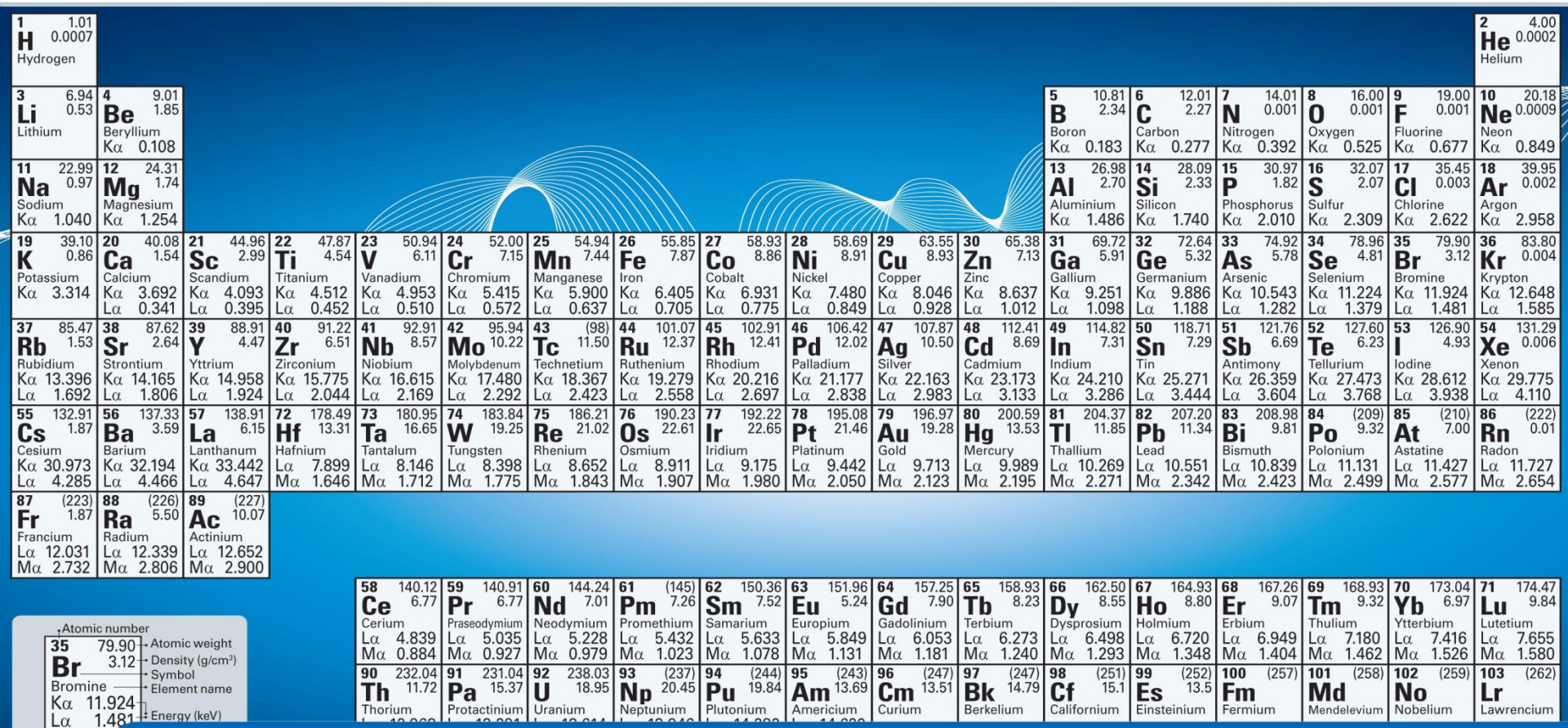
SpectraEDX Training 2014



Outline of Training

1. File structure
2. Setting up the calibration standards
3. Line library
4. Making the calibration
5. Selecting thresholds and transferring cal to instrument

Special Note for Handheld (S1) Users

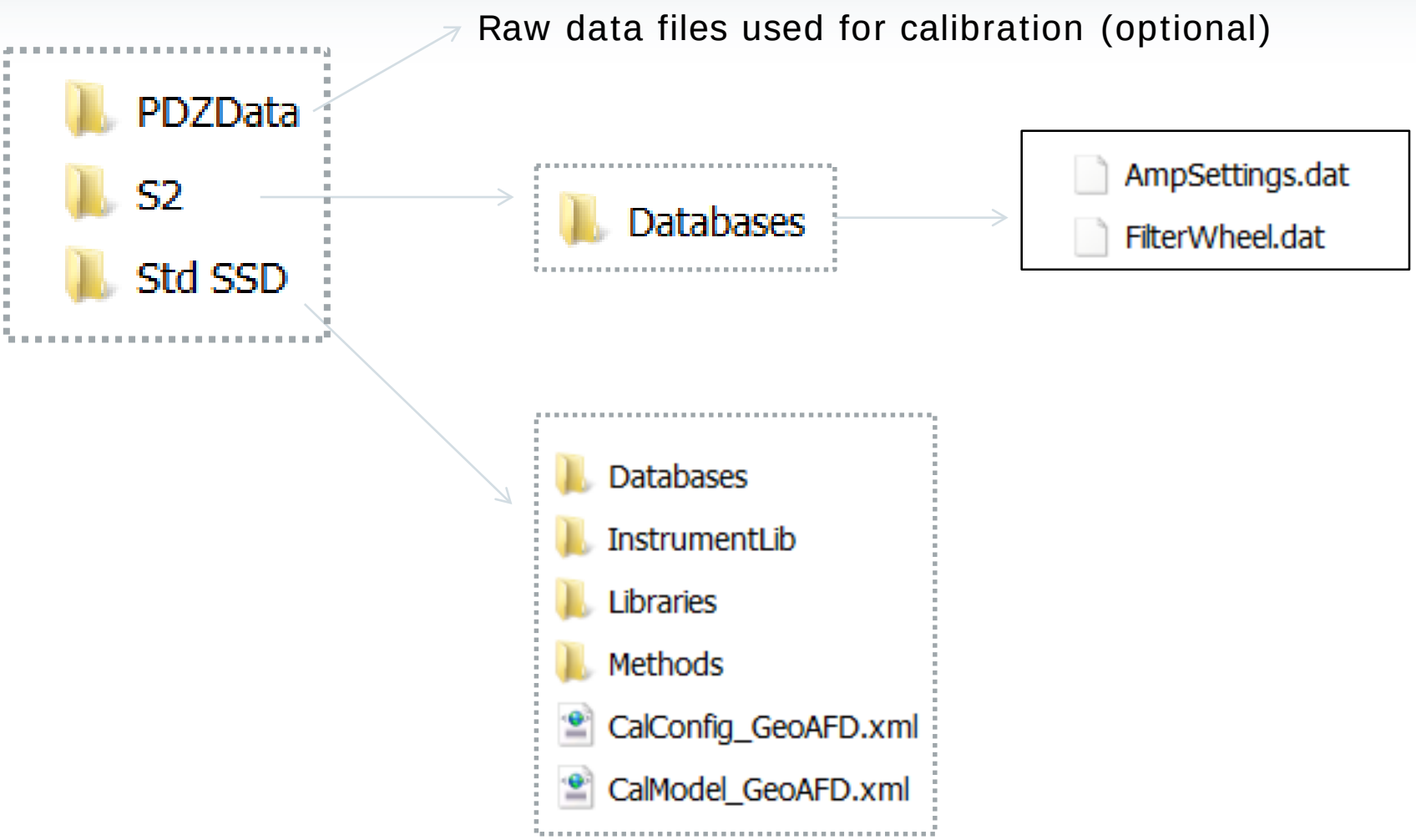
SpectraEDX was designed for use on a computer connected to a single S2 Ranger or other benchtop unit

Some parts of the program are not functional for the S1 handheld instruments, but need to be present in order for the software to work.

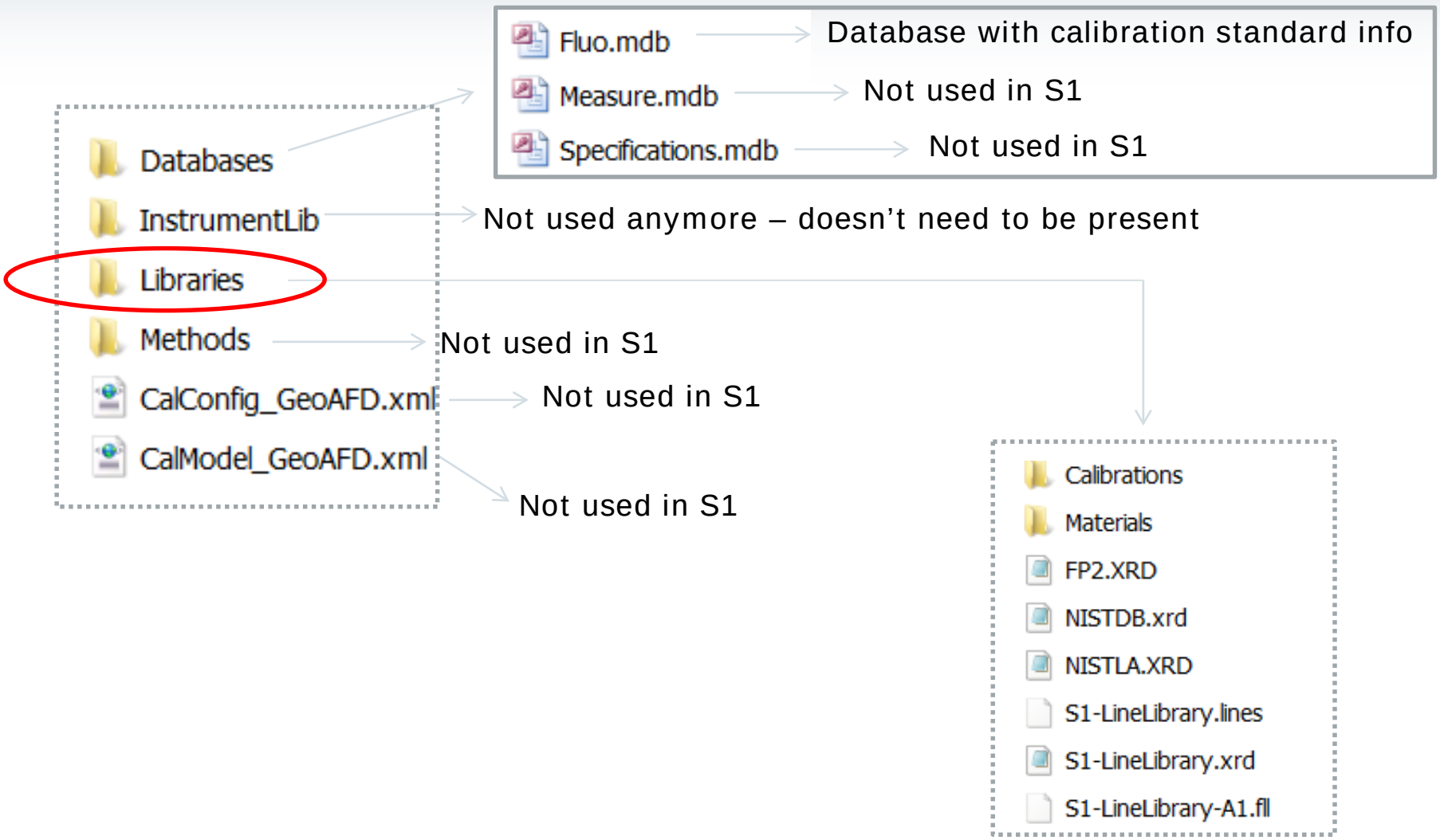
Having multiple SpectraEDX calibration files on one computer requires the use of multiple pointer files or a substitution (S:\) drive.

1. File Structure of SpectraEDX

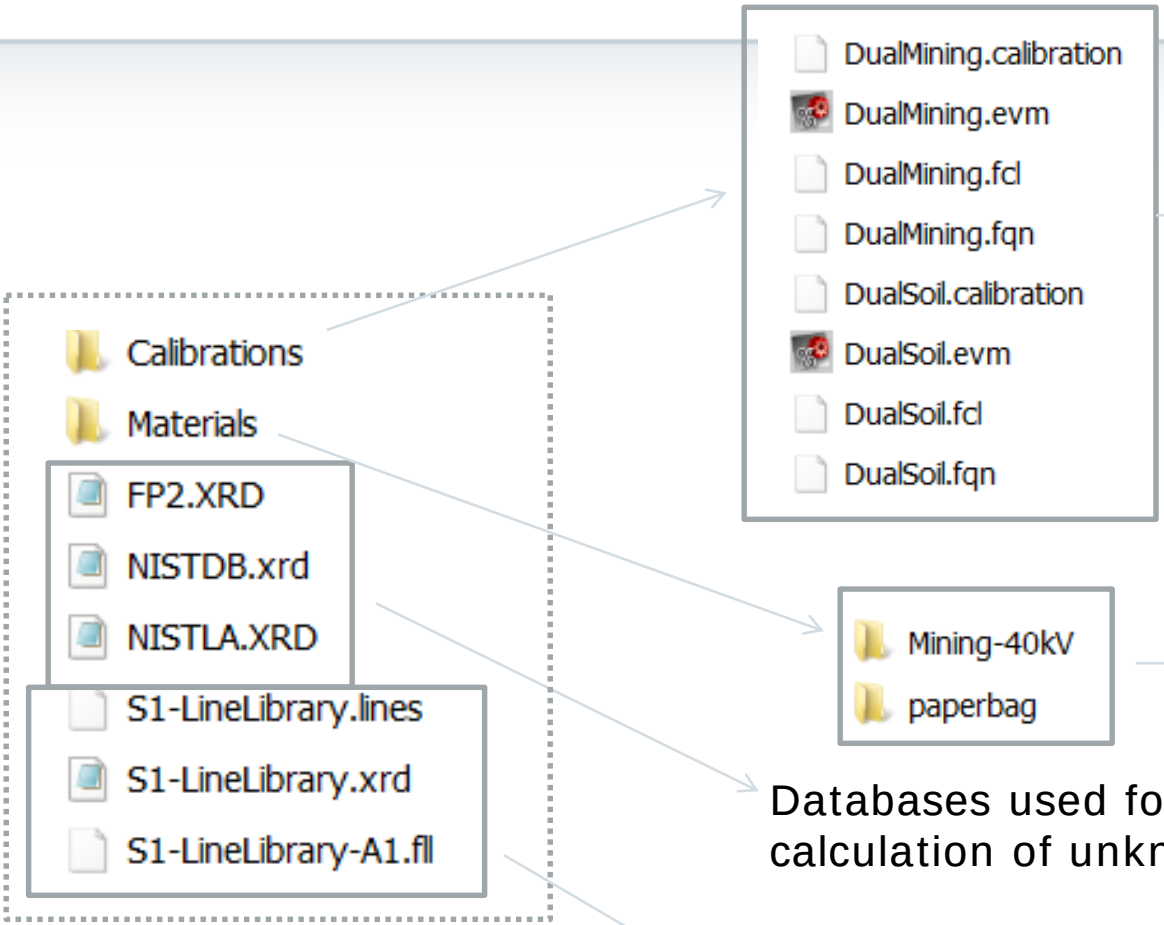
File Structure (part 1) – Top Level Folder



File Structure (part 2) – Mid Level Folders



File Structure (part 3) - Libraries



Evm = evaluation model

Fcl = calibration equations

Fqn = standards info

Calibration = file that is transferred to instrument

Preparations: where standards are stored

Databases used for calculation of unknowns

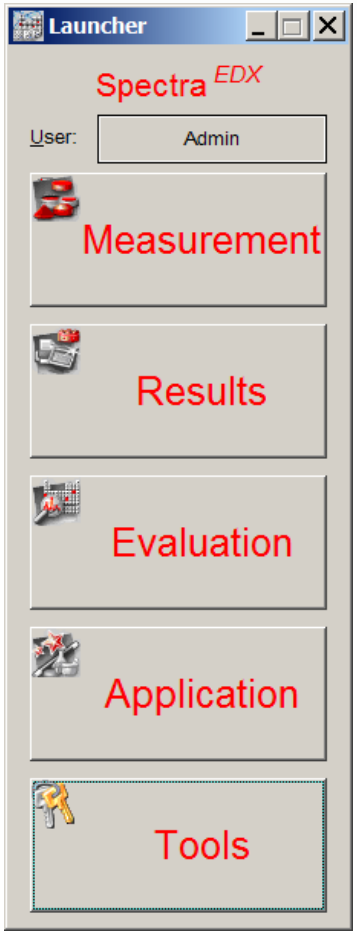
Line libraries: .fll for making calibration, .xrd and .lines for calculation of unknowns

2. Setting up the Calibration Standards

Basic Steps for Defining Calibration Standards

1. Choose material group
2. Choose material
3. Choose elements and compounds
4. Enter names and compositions
5. Choose preparation and size

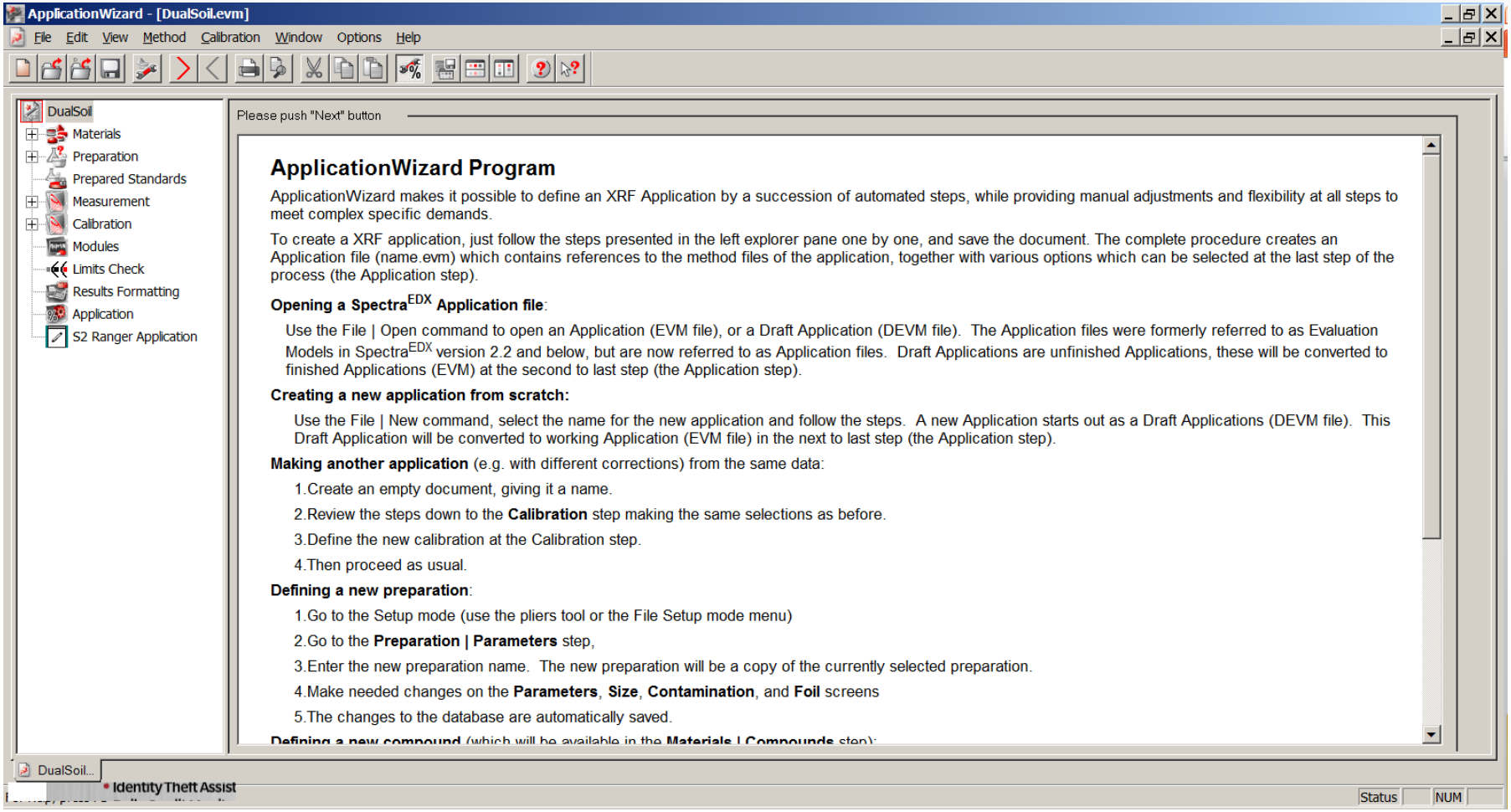
Opening an Application



- Open the toolbox by clicking on the shortcut icon
- Click on the Application button
- Alternately the application can be opened by going to

C:\ProgramFiles(x86)\SpectraEDX\ApplicationWizard.exe

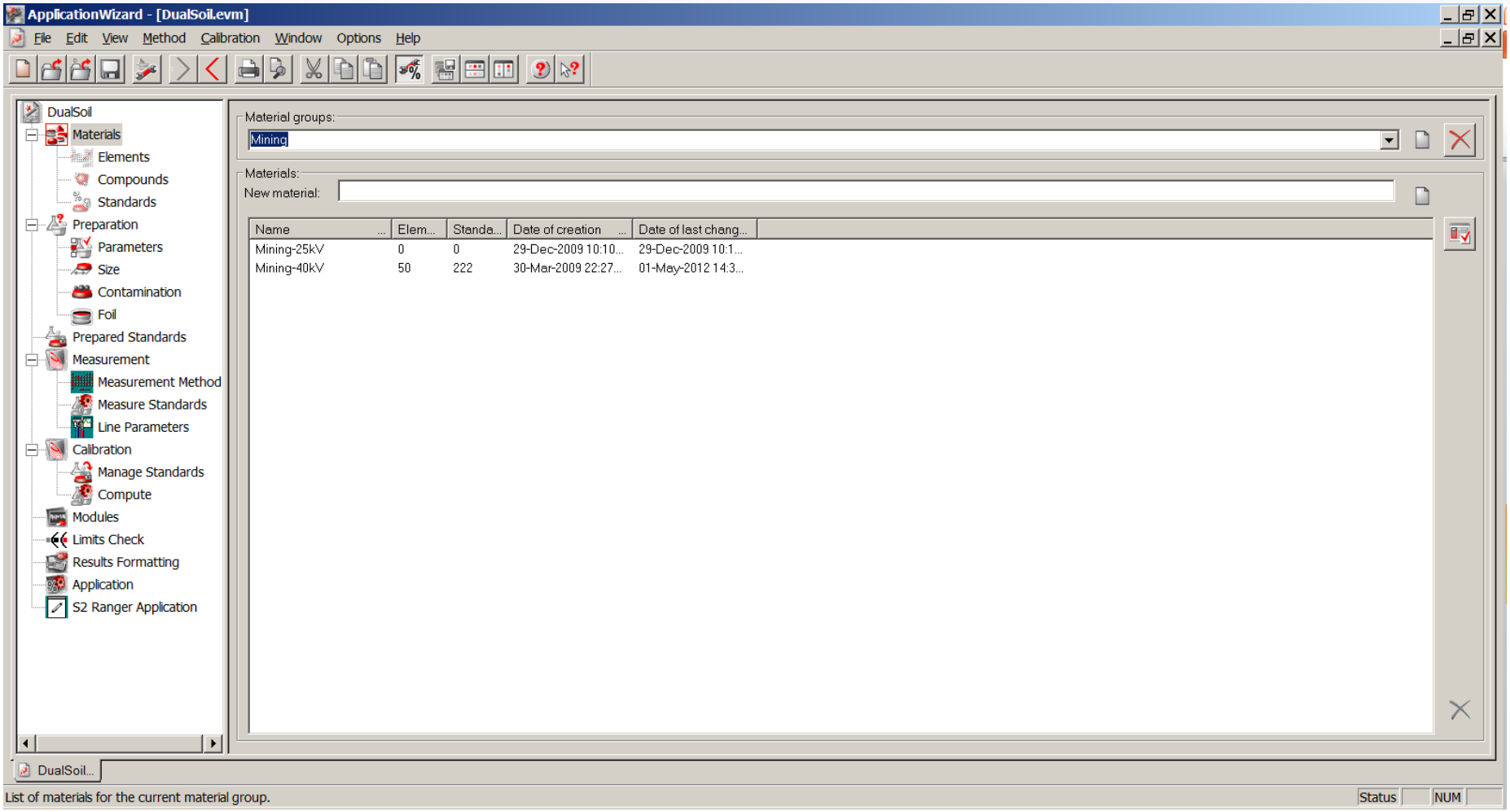
First Screen on Entering SpectraEDX
(new or opened application file)



Calibration “Tree” List

Expanded

Materials Page – choose material group and material



Material Group

A Material Group is a set of Materials that all have something in common. They can be categorized into material types (metals, geo, etc.), customer names, project types, or a single Material Group can be used for everything.

In the above slide, the Material Group is Mining, and it contains two Materials: Mining-25kV and Mining-40kV. (In this example, only Mining-40kV is populated in the database, so the Mining-25kV Material shows no standards.)

The Material and Material Group information is stored in the Fluo.mdb database.

Additives and Contaminants are separate Material Groups.

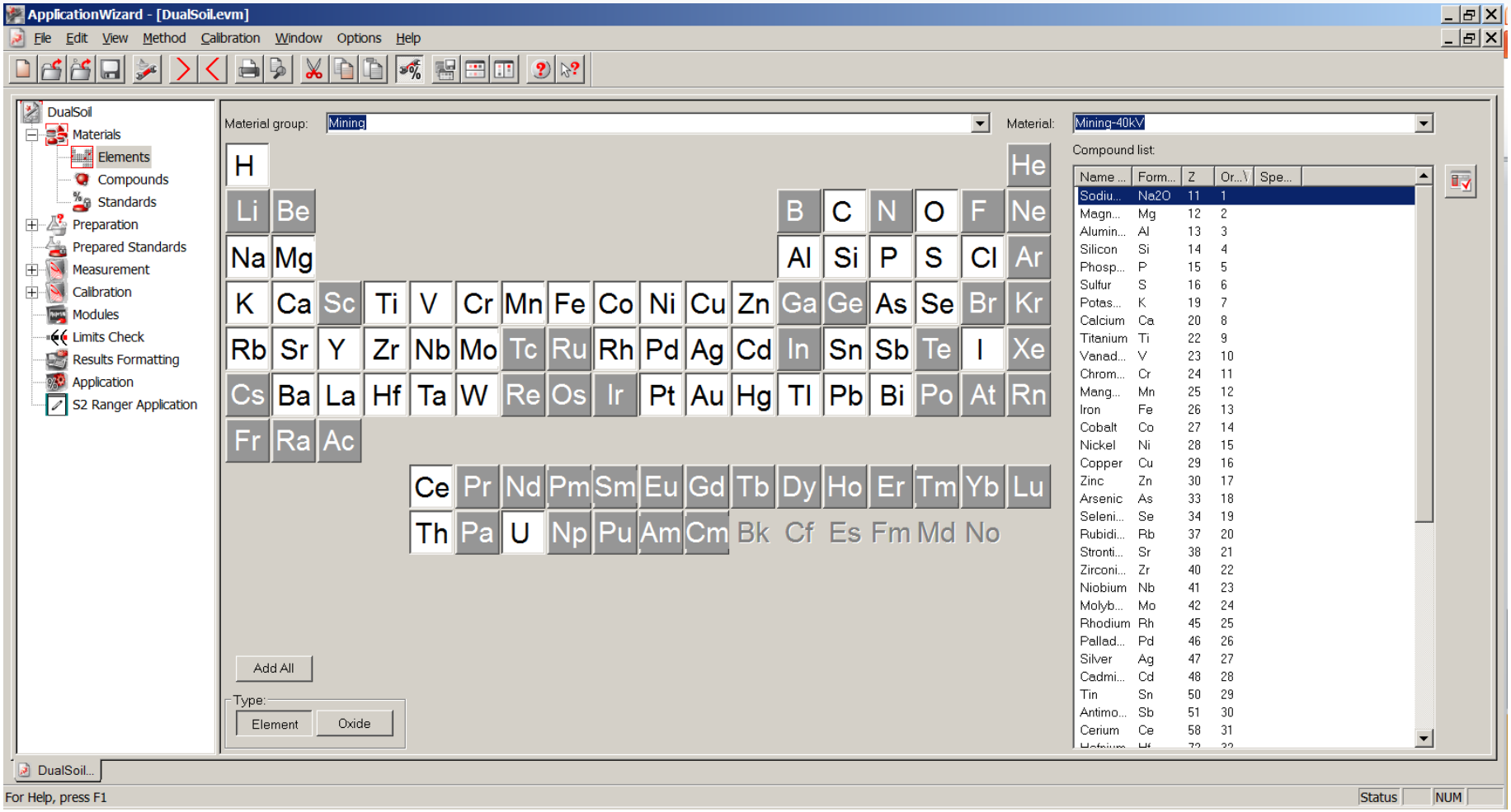
Material

A Material is a set of standards that are used in a particular calibration or set of calibrations. Standards with exactly the same name cannot be used in different Materials.

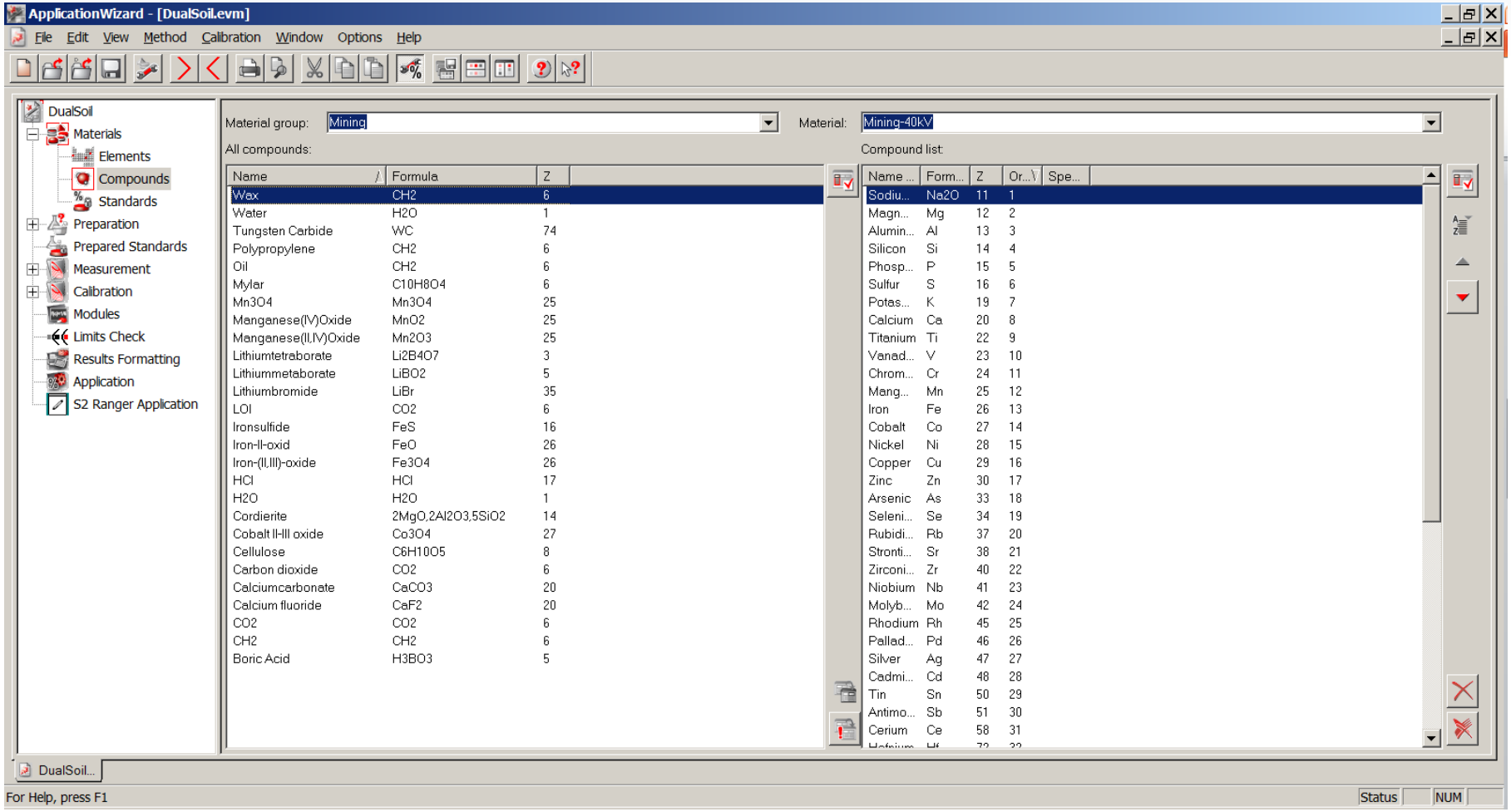
Our naming conventions:
In the two Materials mentioned above, standards in Mining-25kV begin with M25 and in Mining-40kV begin with M40.

For example, SRM2710 would be called M25SRM2710 in one Material and M40SRM2710 in the other.

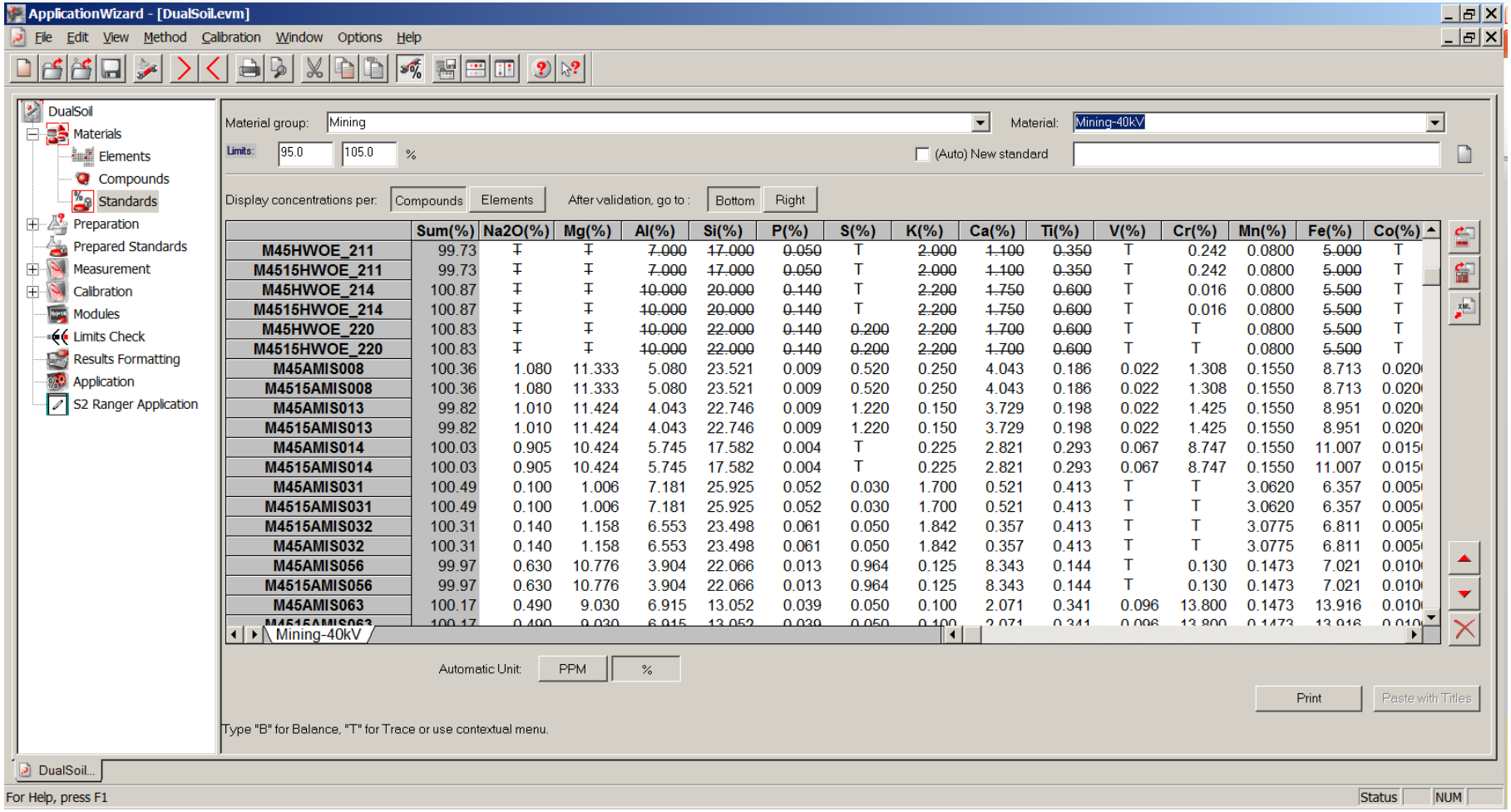
Choosing Elements in the Material



Choosing Compounds in the Material



Inputting Names and Data for Standards



	Sum(%)	Na2O(%)	Mg(%)	Al(%)	Si(%)	P(%)	S(%)	K(%)	Ca(%)	Ti(%)	V(%)	Cr(%)	Mn(%)	Fe(%)	Co(%)
M45HWOE_211	99.73	T	T	7.000	17.000	0.050	T	2.000	1.100	0.350	T	0.242	0.0800	5.000	T
M4515HWOE_211	99.73	T	T	7.000	17.000	0.050	T	2.000	1.100	0.350	T	0.242	0.0800	5.000	T
M45HWOE_214	100.87	T	T	10.000	20.000	0.140	T	2.200	1.750	0.600	T	0.016	0.0800	5.500	T
M4515HWOE_214	100.87	T	T	10.000	20.000	0.140	T	2.200	1.750	0.600	T	0.016	0.0800	5.500	T
M45HWOE_220	100.83	T	T	10.000	22.000	0.140	0.200	2.200	1.700	0.600	T	T	0.0800	5.500	T
M4515HWOE_220	100.83	T	T	10.000	22.000	0.140	0.200	2.200	1.700	0.600	T	T	0.0800	5.500	T
M45AMIS008	100.36	1.080	11.333	5.080	23.521	0.009	0.520	0.250	4.043	0.186	0.022	1.308	0.1550	8.713	0.020
M4515AMIS008	100.36	1.080	11.333	5.080	23.521	0.009	0.520	0.250	4.043	0.186	0.022	1.308	0.1550	8.713	0.020
M45AMIS013	99.82	1.010	11.424	4.043	22.746	0.009	1.220	0.150	3.729	0.198	0.022	1.425	0.1550	8.951	0.020
M4515AMIS013	99.82	1.010	11.424	4.043	22.746	0.009	1.220	0.150	3.729	0.198	0.022	1.425	0.1550	8.951	0.020
M45AMIS014	100.03	0.905	10.424	5.745	17.582	0.004	T	0.225	2.821	0.293	0.067	8.747	0.1550	11.007	0.015
M4515AMIS014	100.03	0.905	10.424	5.745	17.582	0.004	T	0.225	2.821	0.293	0.067	8.747	0.1550	11.007	0.015
M45AMIS031	100.49	0.100	1.006	7.181	25.925	0.052	0.030	1.700	0.521	0.413	T	T	3.0620	6.357	0.005
M4515AMIS031	100.49	0.100	1.006	7.181	25.925	0.052	0.030	1.700	0.521	0.413	T	T	3.0620	6.357	0.005
M4515AMIS032	100.31	0.140	1.158	6.553	23.498	0.061	0.050	1.842	0.357	0.413	T	T	3.0775	6.811	0.005
M45AMIS032	100.31	0.140	1.158	6.553	23.498	0.061	0.050	1.842	0.357	0.413	T	T	3.0775	6.811	0.005
M45AMIS056	99.97	0.630	10.776	3.904	22.066	0.013	0.964	0.125	8.343	0.144	T	0.130	0.1473	7.021	0.010
M4515AMIS056	99.97	0.630	10.776	3.904	22.066	0.013	0.964	0.125	8.343	0.144	T	0.130	0.1473	7.021	0.010
M45AMIS063	100.17	0.490	9.030	6.915	13.052	0.039	0.050	0.100	2.071	0.341	0.096	13.800	0.1473	13.916	0.010

Rules for Inputting Standards

1. All standard names must be typed in manually (there is one exception to this: “paste with titles”)

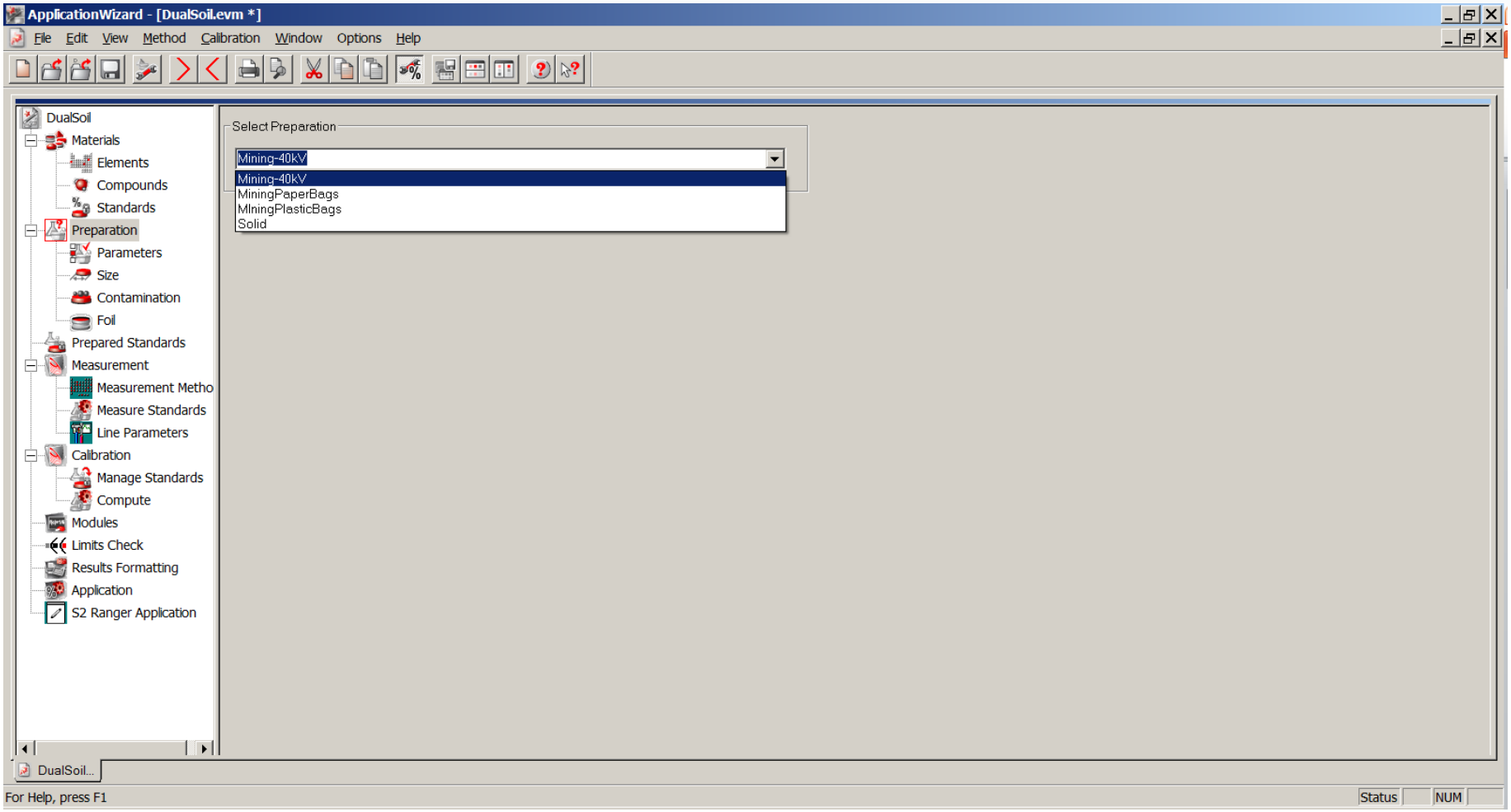
2. Values can either be typed manually or input from a spreadsheet

3. Values can be output to a spreadsheet

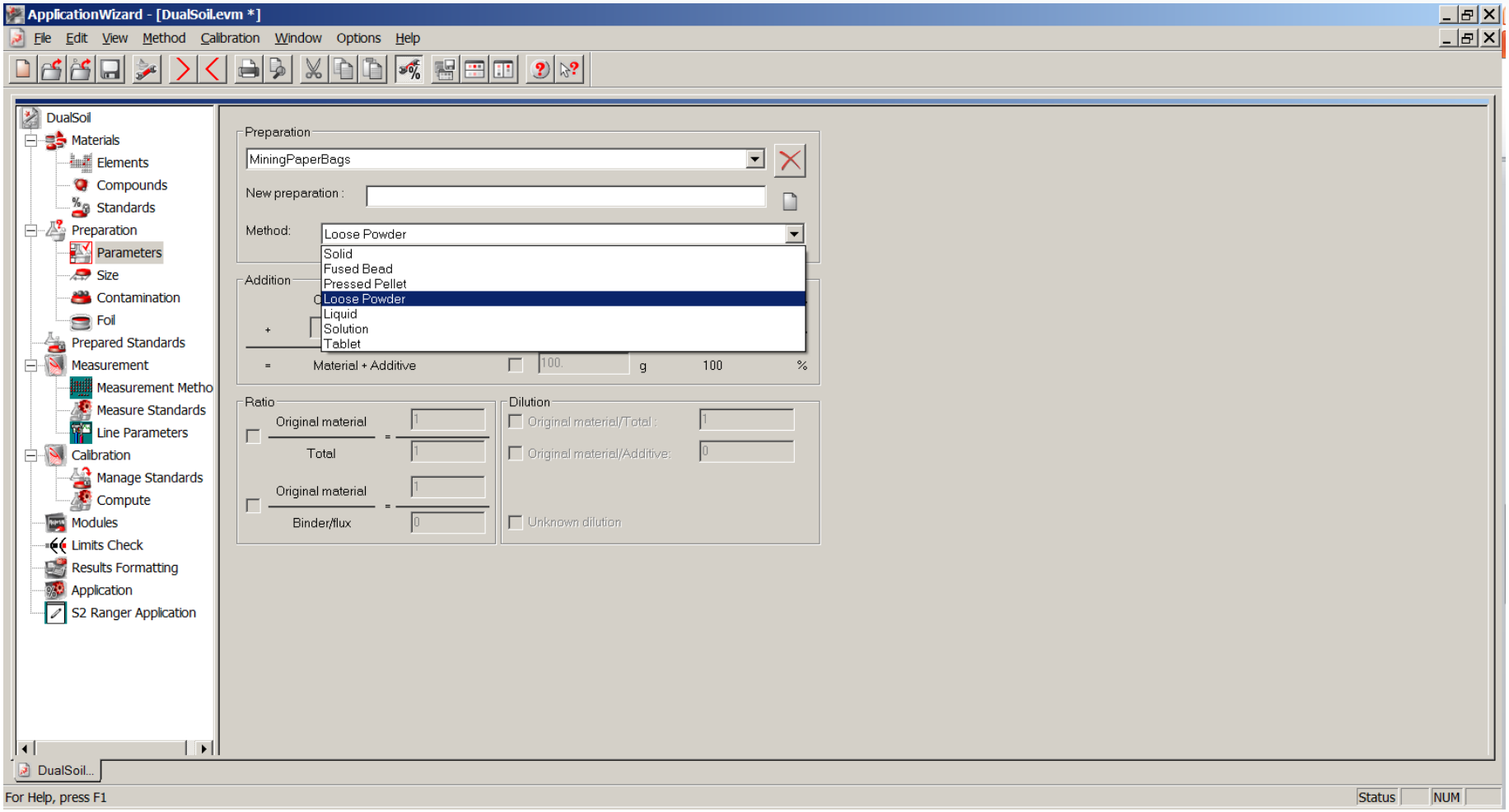
4. Tools are available such as ppm/%, “inaccurate”, column balance, and line balance

5. Concentrations must add to 100% (within limits at top) to be used with FP-based calibrations

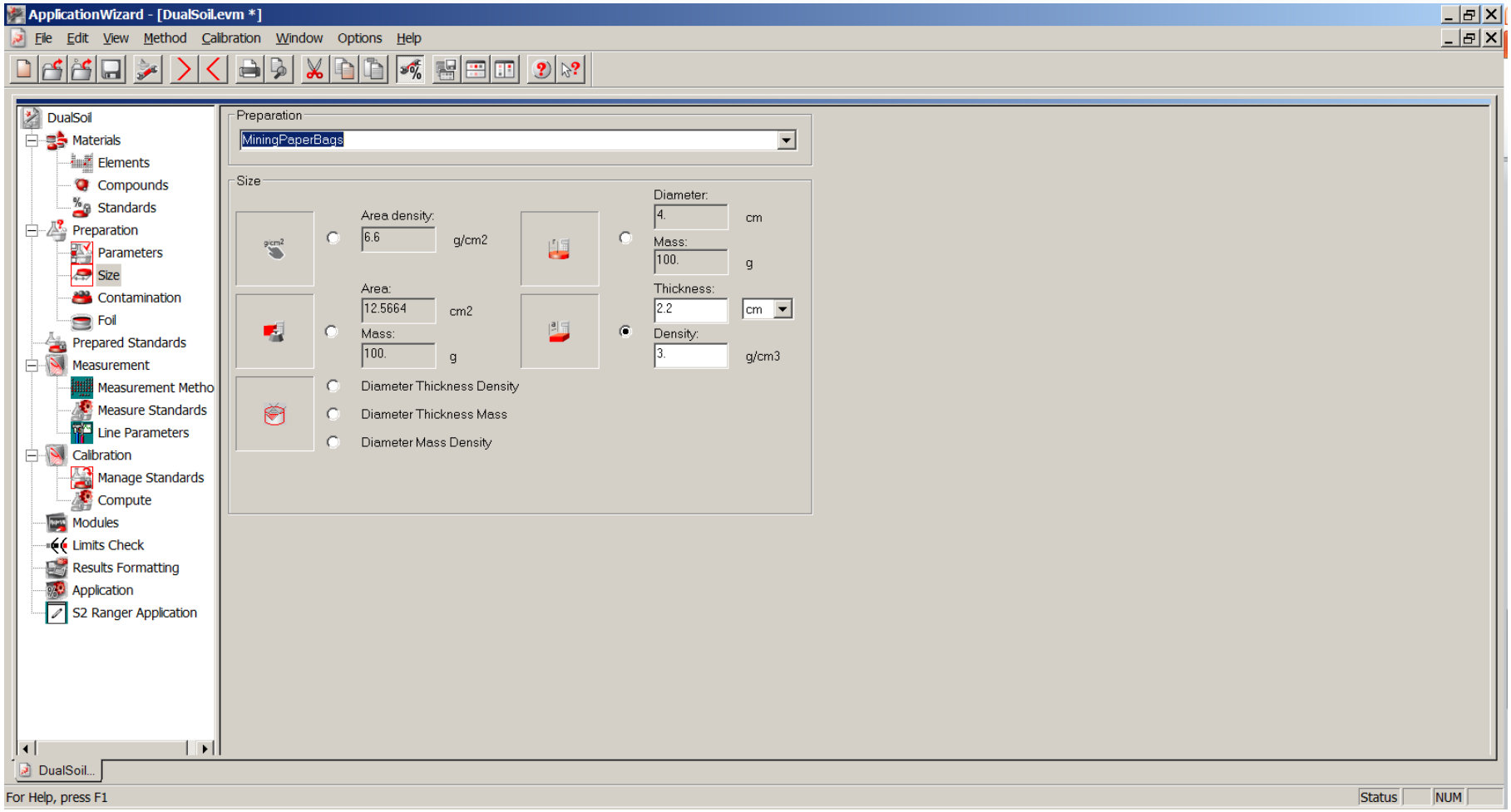
Selecting a Preparation for a Material



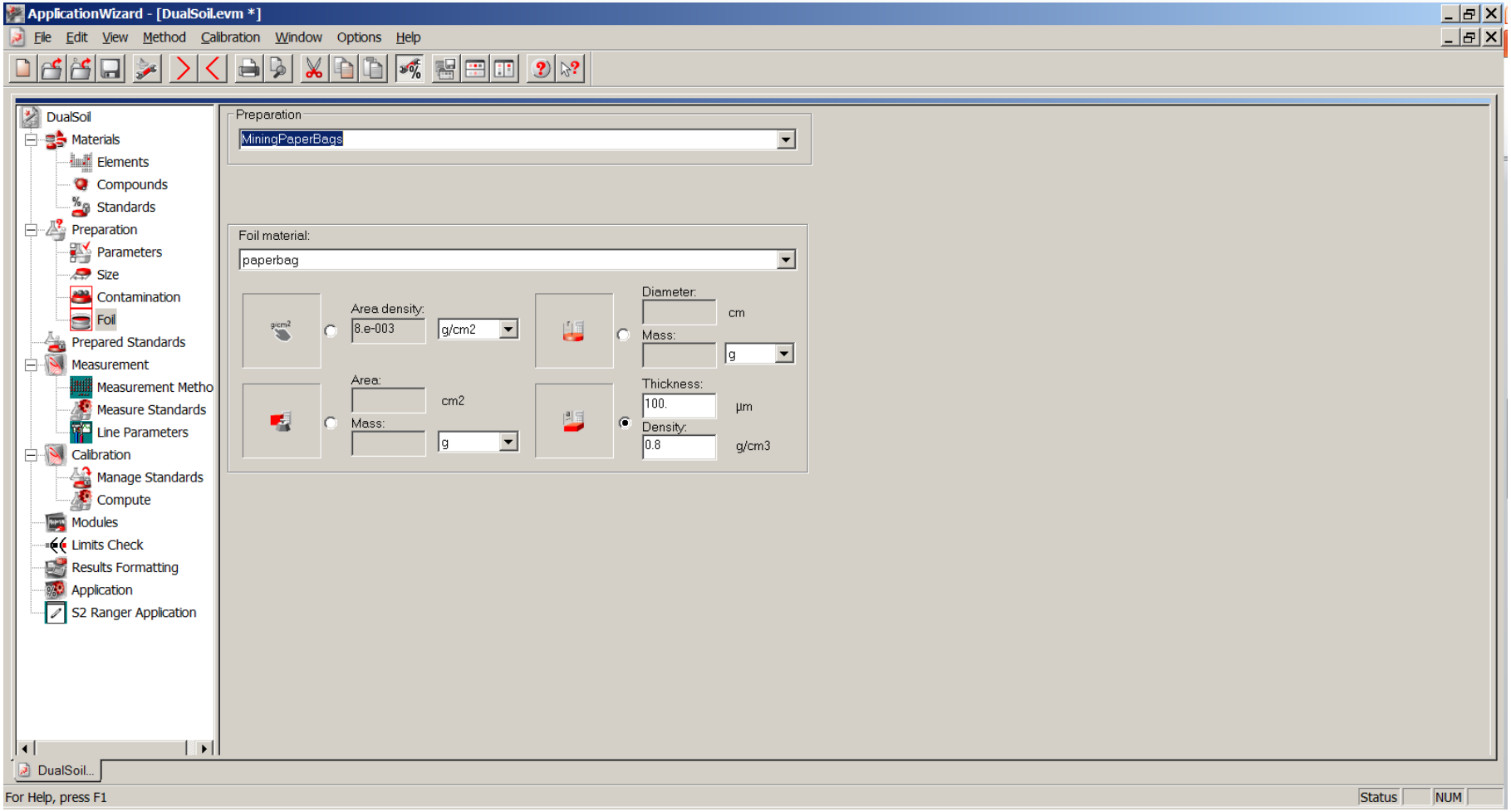
Defining a Preparation



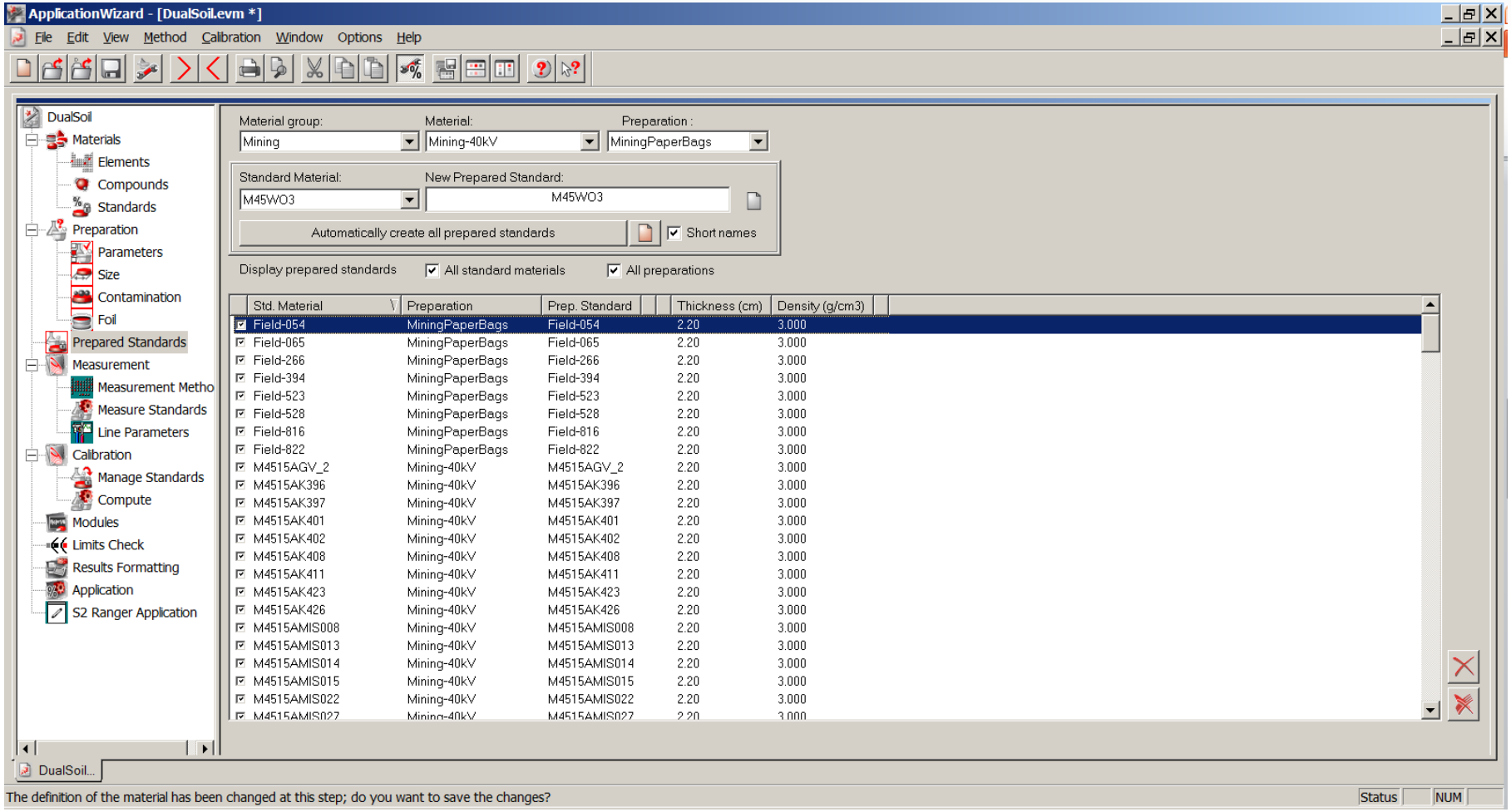
Infinite Thickness Calculation



“Foil” Attenuation Definition



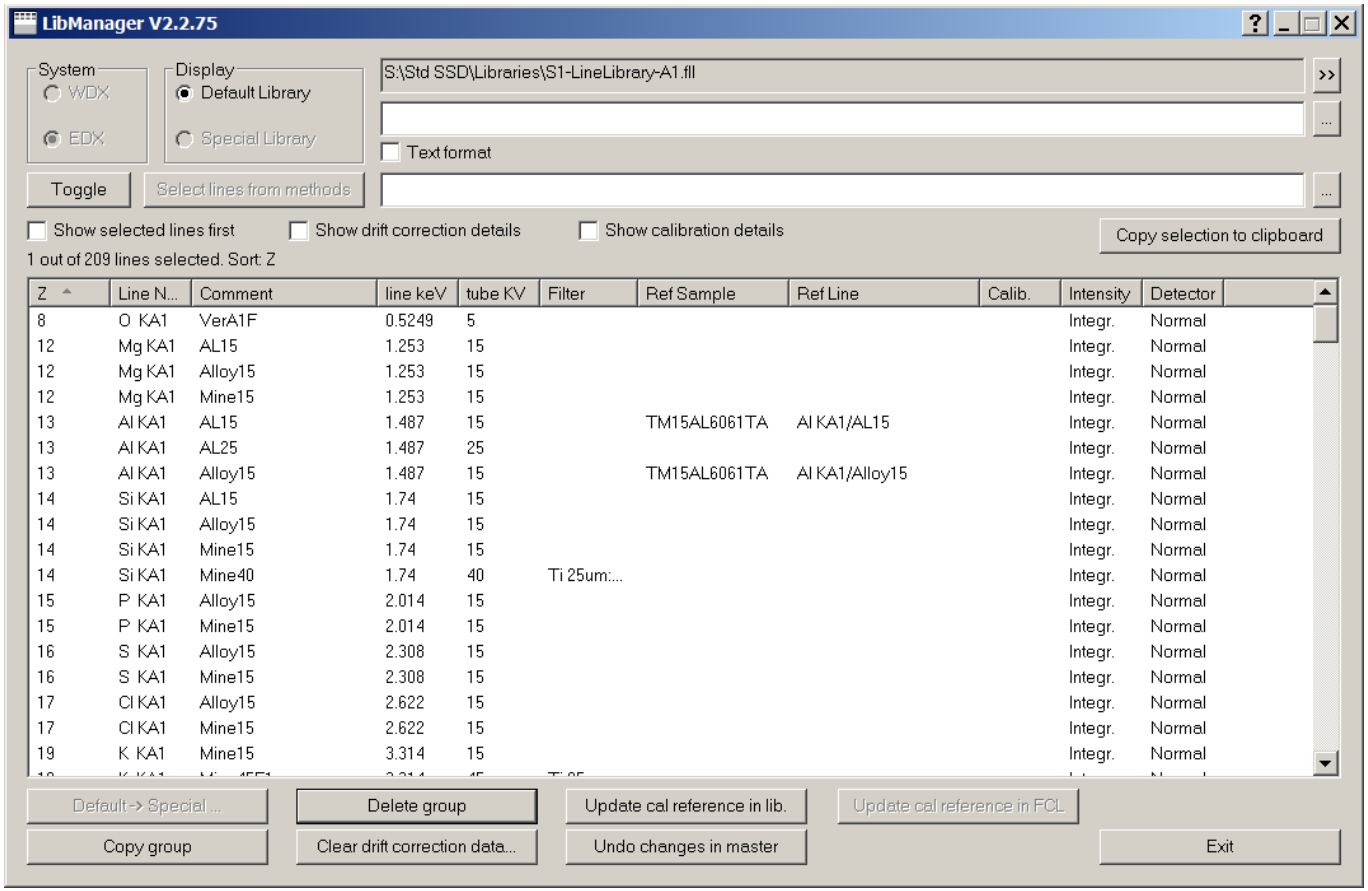
Choosing the Prepared Standards



3. Using and editing the Line Library

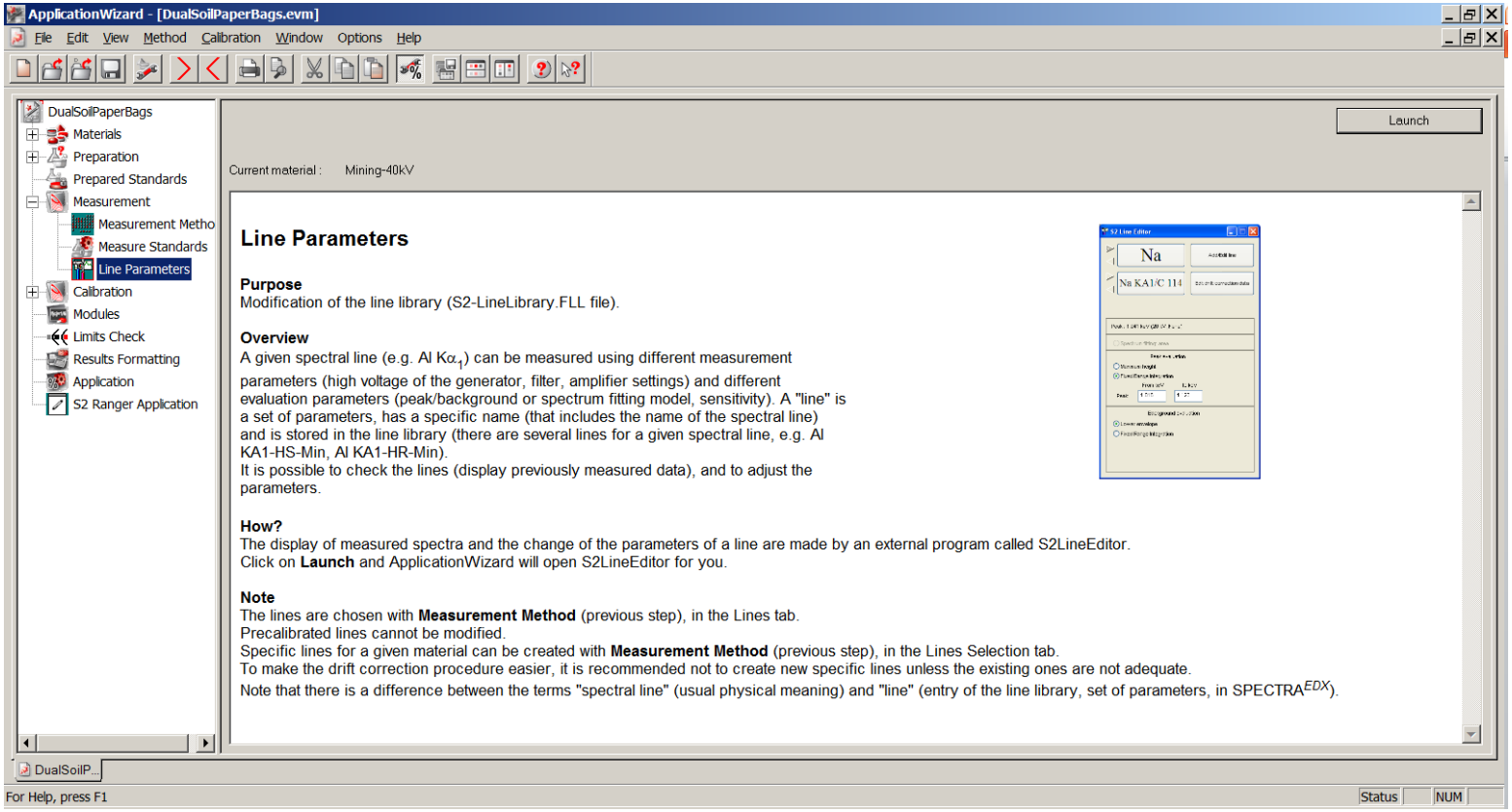
Line Library Access #1

Launcher: Tools → Line Library Maintenance



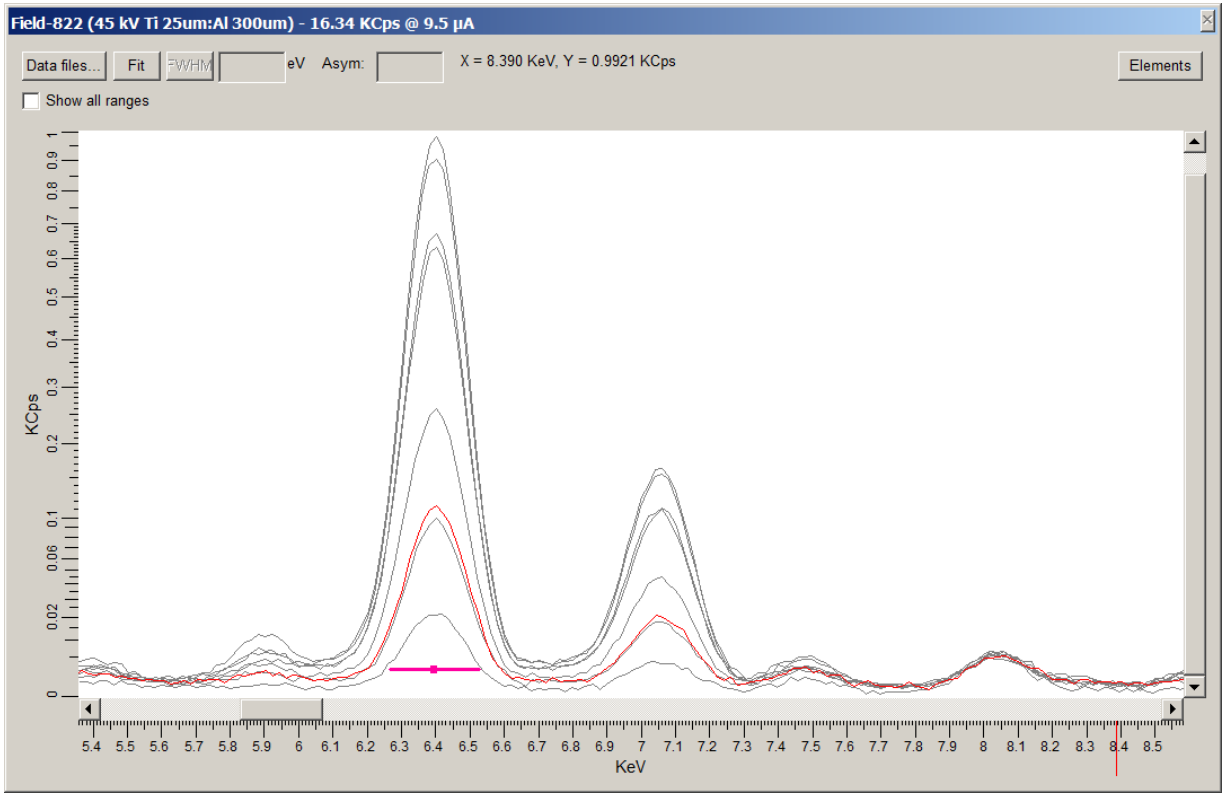
Line Library Access #2

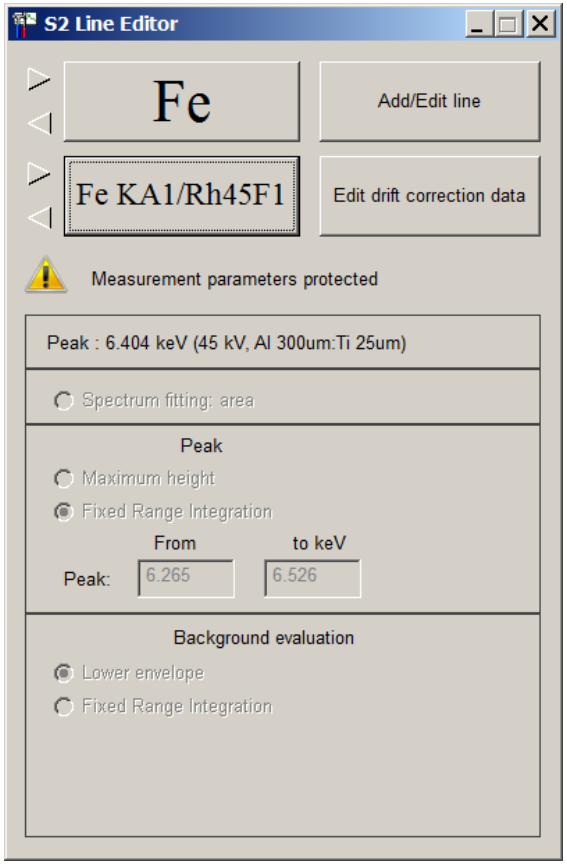
In application → Measurement section → Line Parameters
Click on Launch



Line Editor Interface

Choose element and line to edit or check
Pink line in graph is linewidth





Line Editor Hints

- Line chosen must have same voltage and filter as the calibration measurements
- Lines must be unlocked before editing
- For most cases, Fixed Range Integration with Lower Envelope background evaluation is the correct type of peak to use
- Occasionally Fixed Range Integration background is useful
- Spectrum fitting mode is not active for the handhelds
- See S2LineEditor training material for more information

More Line Editor Hints

- Some lines have drift correction data. This is used in the benchtop (S2) units to correct for intensity drift in detectors. For handheld (S1) units, intensity drift is negligible. Drift correction in SpectraEDX is only used to transfer calibrations between instruments, and currently only works for some situations.

- To edit a line, it must be unlocked, which is done by right-clicking on the top grey area and choosing “unlock all lines”. The pink line on the graph can then be changed or new limits typed in.

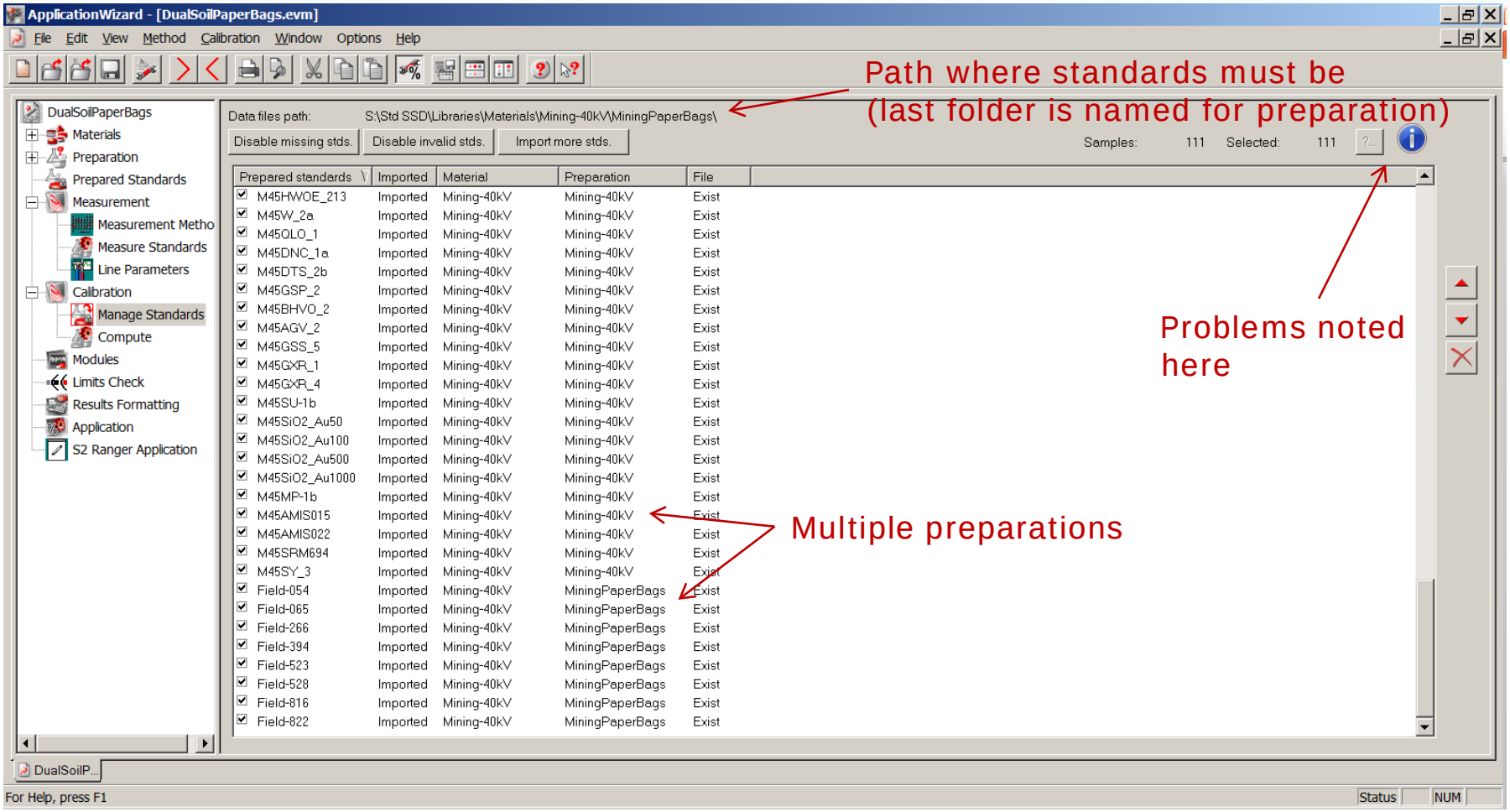
- Adding a new line is done by clicking “insert foreign line” in the same drop-down menu.

3. Creating the Calibration

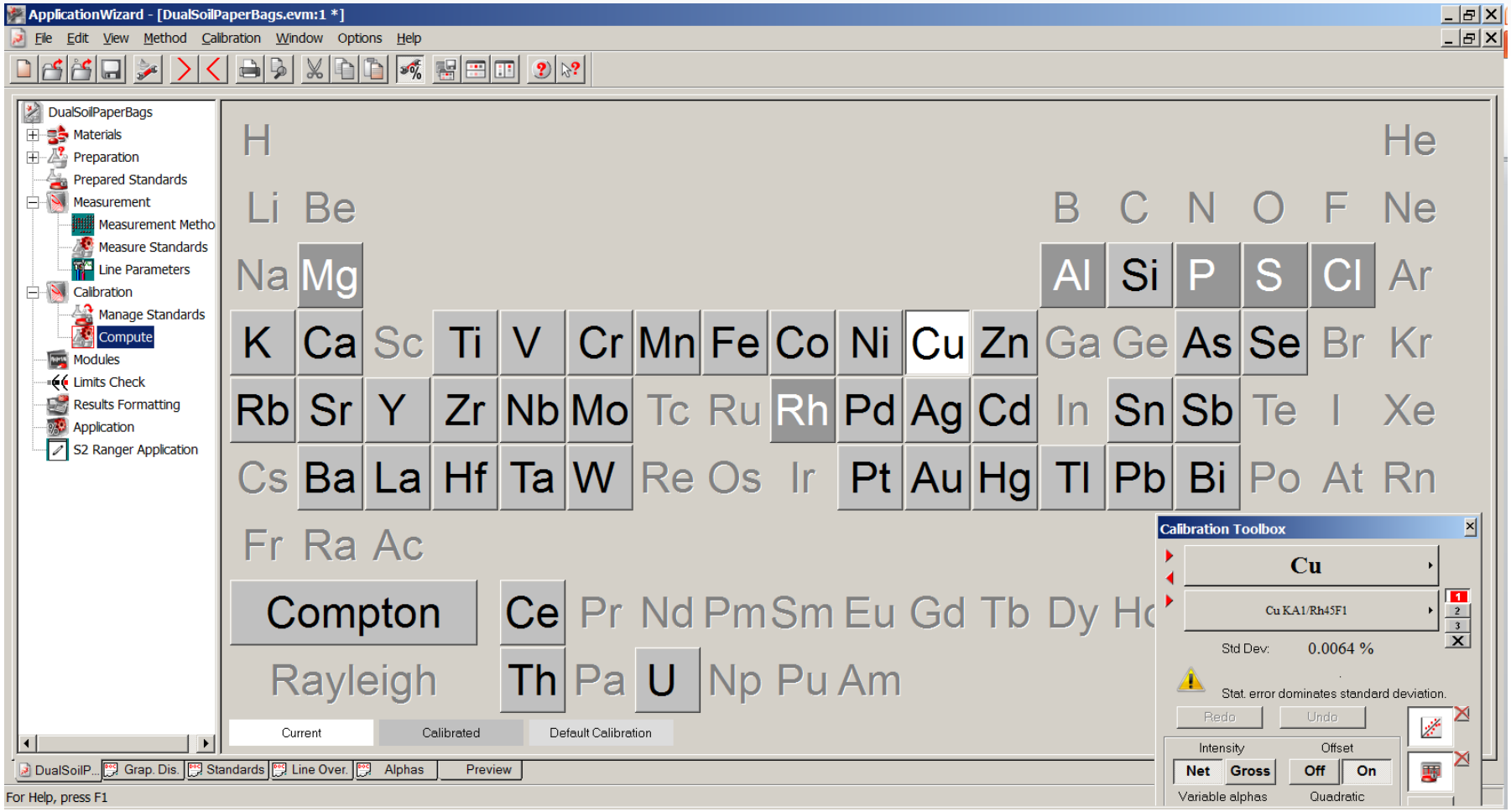
Basic Calibration Steps

1. Choose standards
2. Determine necessary overlaps
3. Determine appropriate matrix coefficients

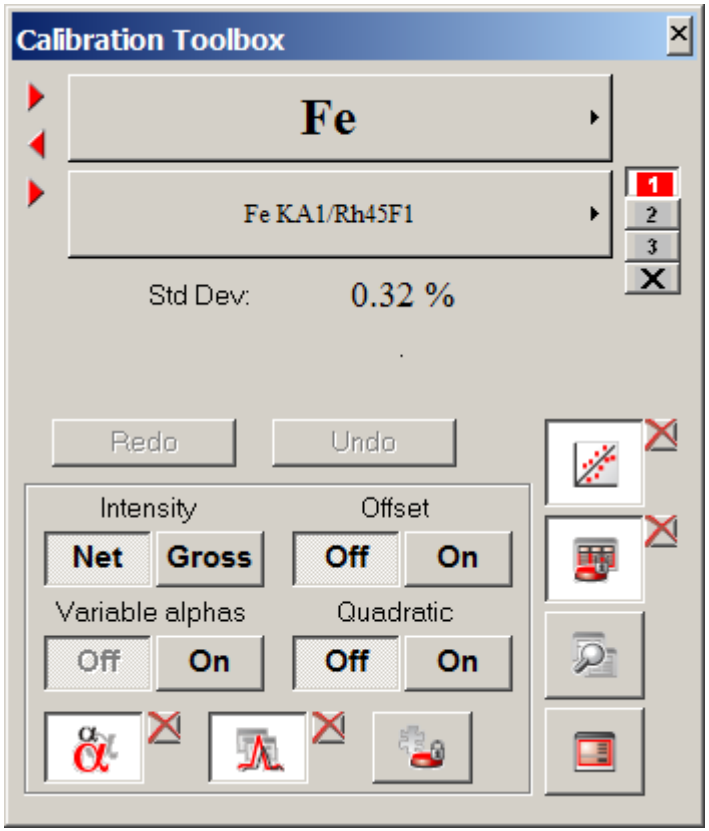
Choosing Standards



Elements Screen with Toolbox



Toolbox Functions

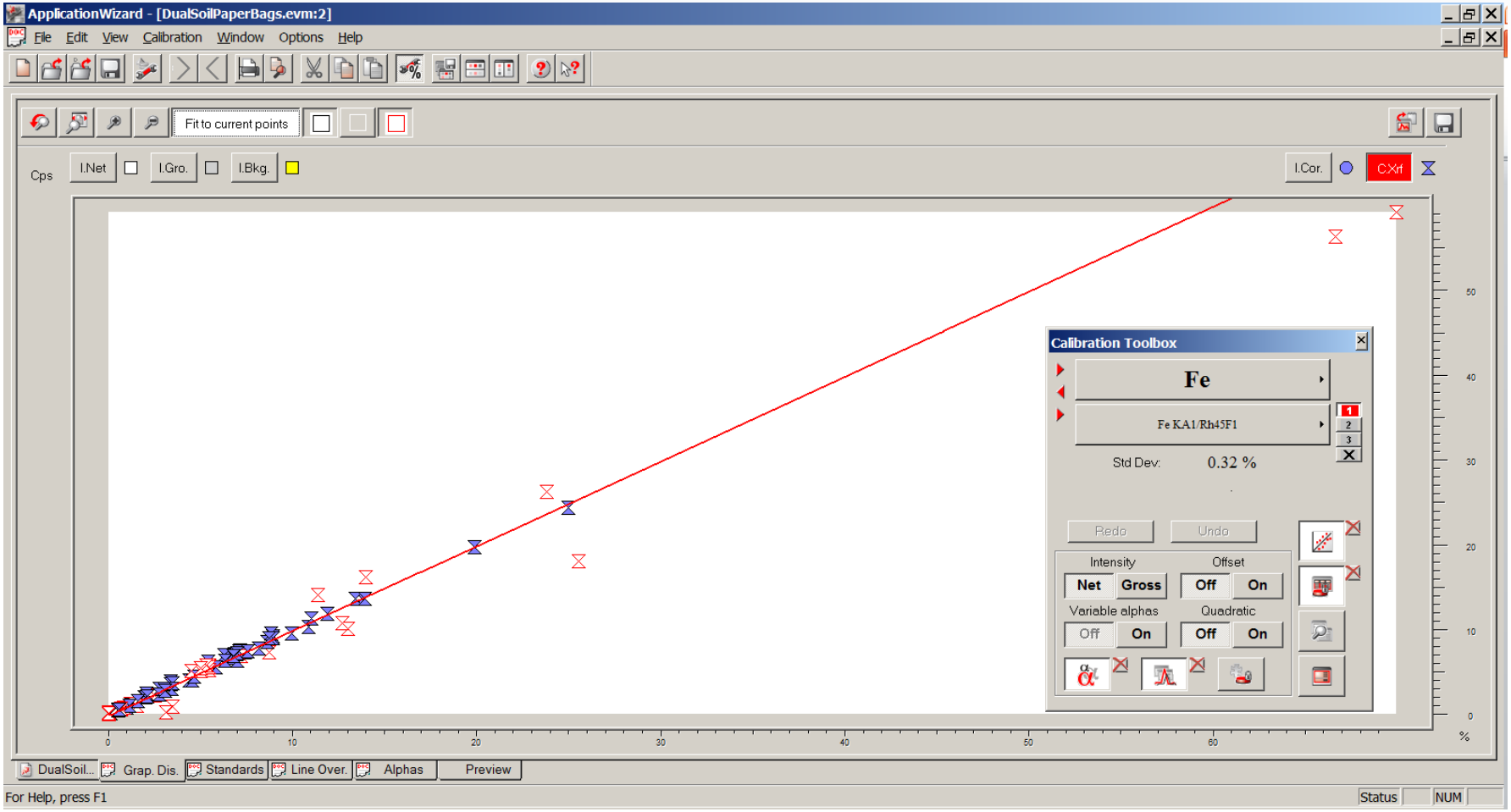


- Switch between screens
- Control offset and quadratic
- Undo/redo
- Control element and line used
- Monitor standard deviation

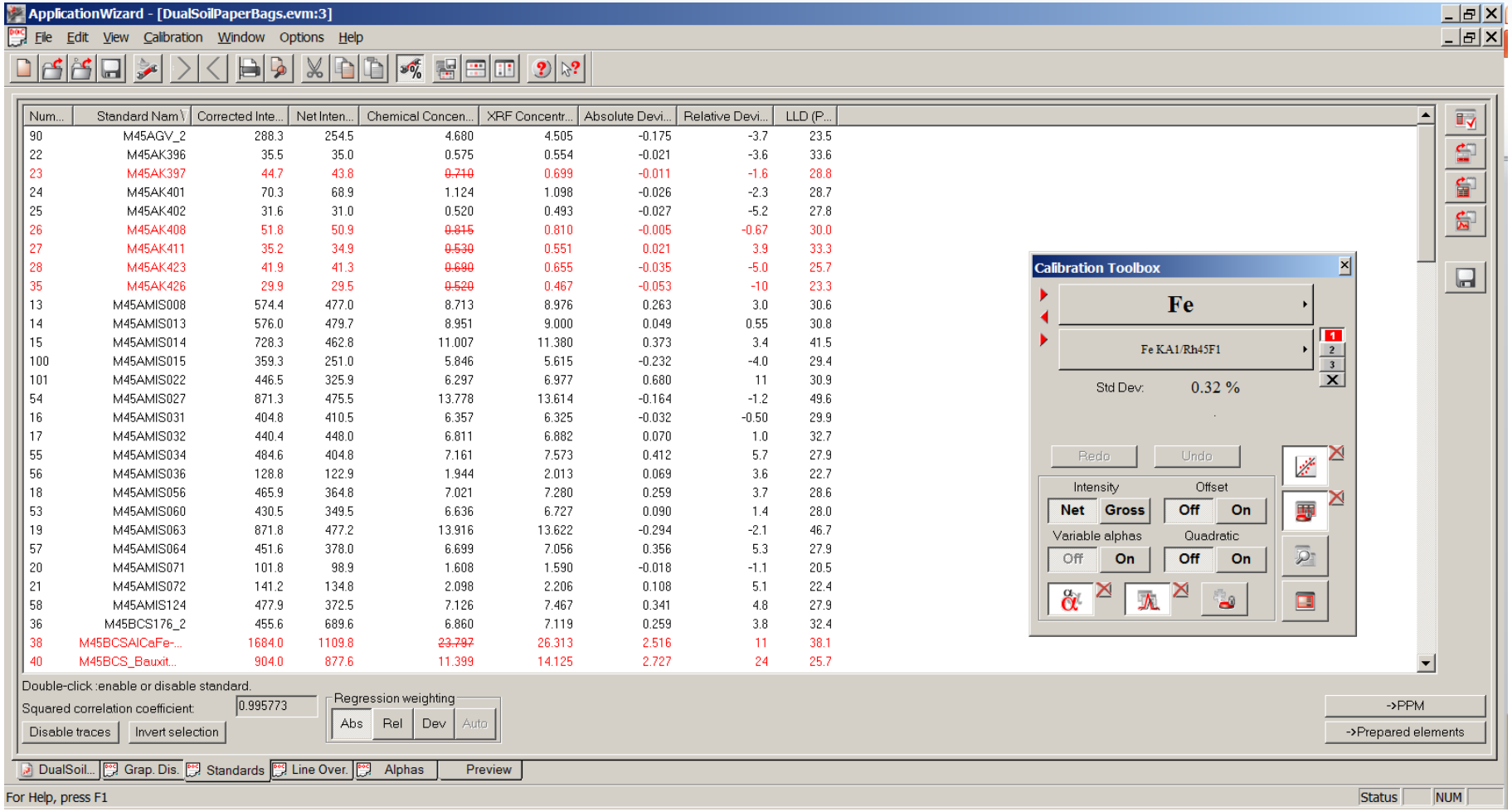
Available Screens

- Alphas
- Overlaps
- Internal standard
- Graph
- Alphas
- Tabular display
- Summary

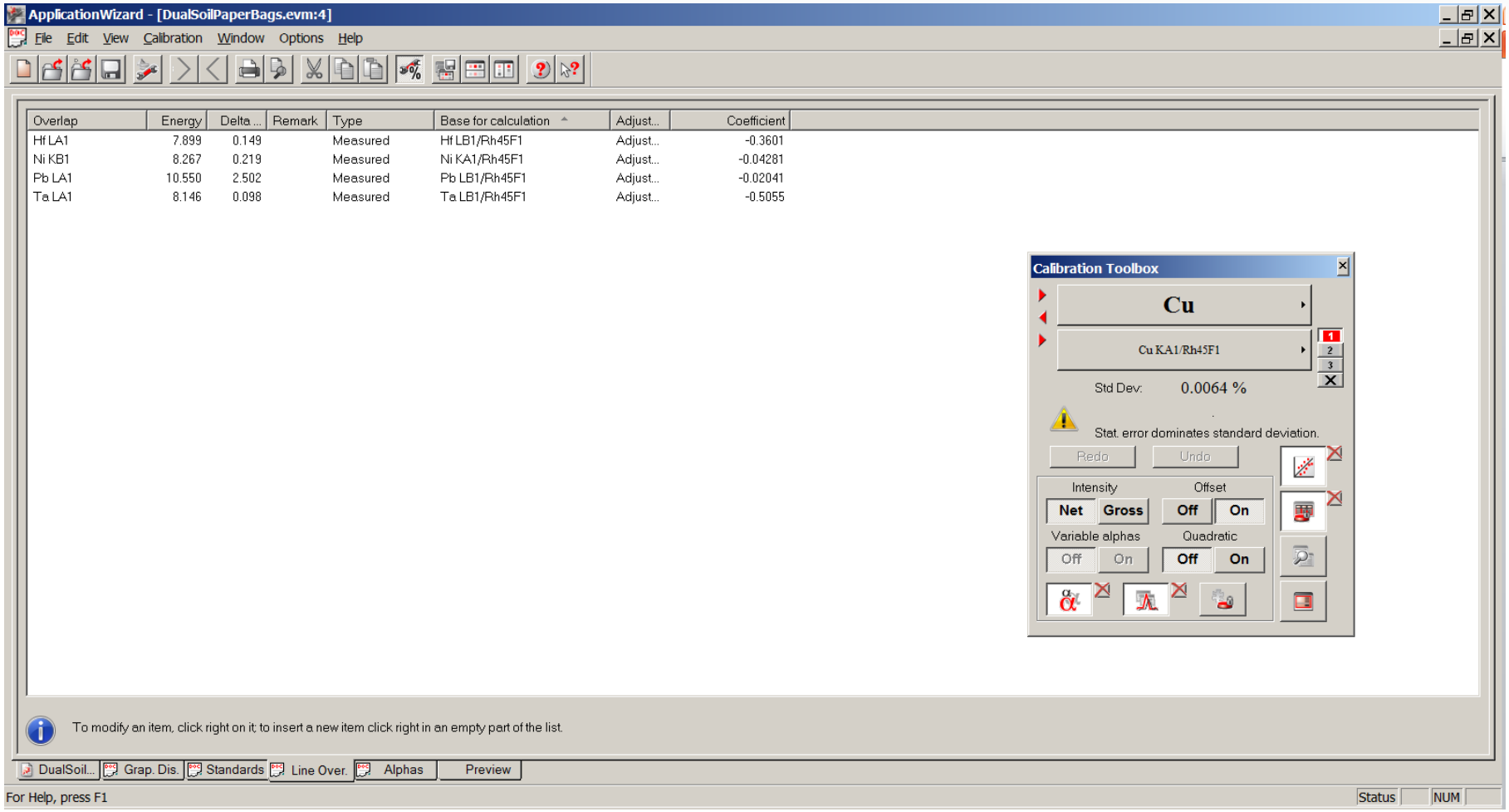
Graph Screen with Toolbox



Standards (Tabular Display) Screen with Toolbox

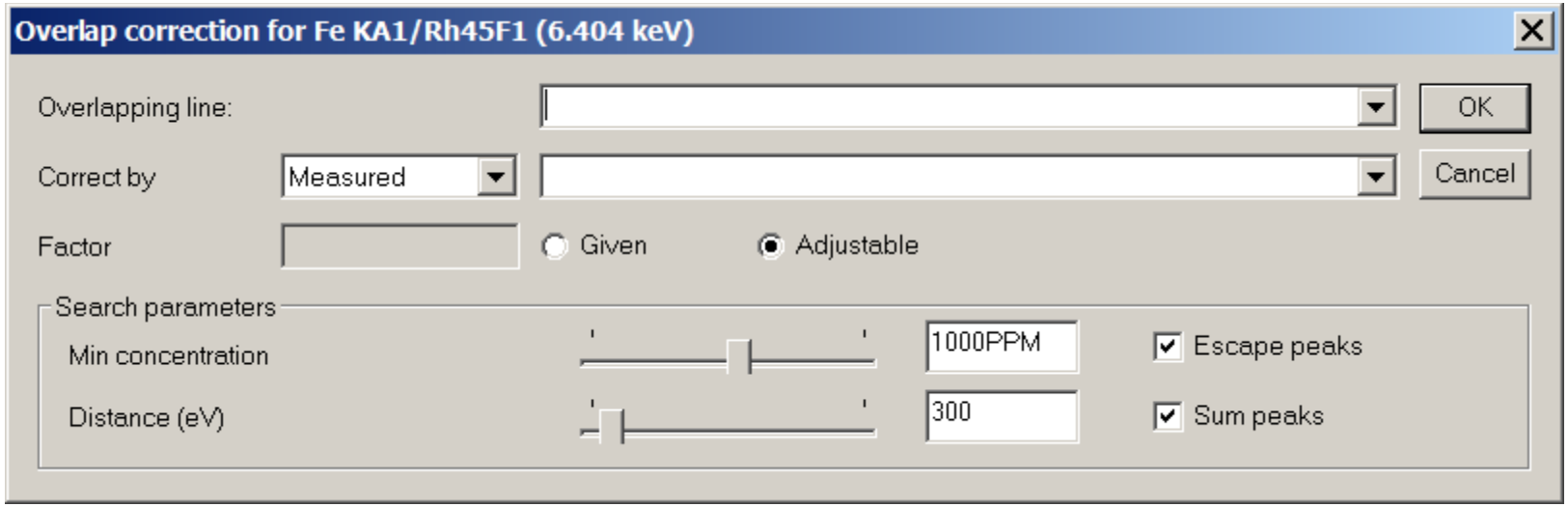


Overlaps Screen with Toolbox

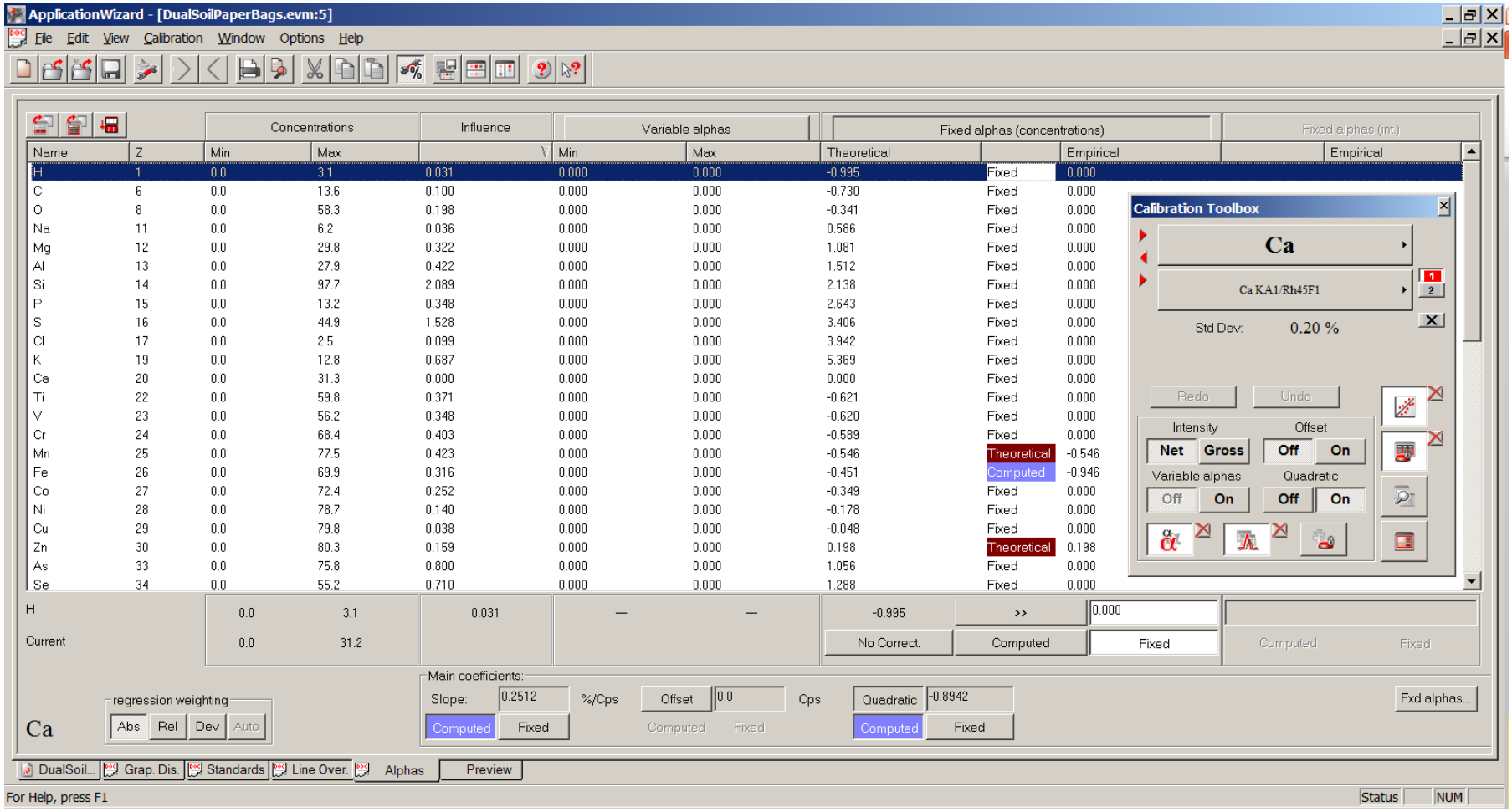


Adding an Overlap

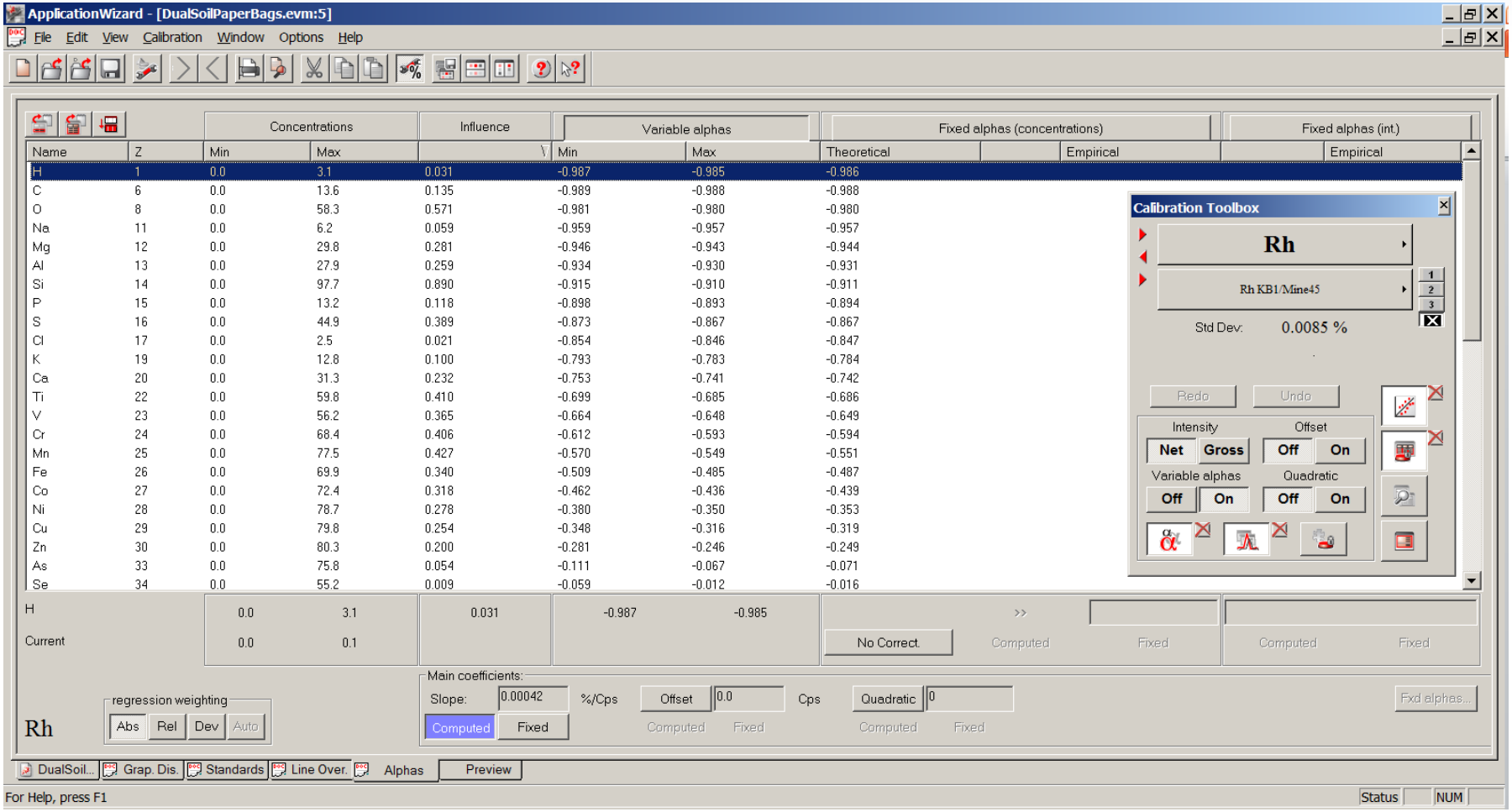
- Right click anywhere on Overlaps screen to get this box
- Enter overlapping line or choose from drop-down menu
- Choose correction method (measured, calculated, concentration)
- Click OK and it will be added to the list
- Escape and sum peaks can be included in the list or excluded



Alphas Screen with Fixed Alphas



Alphas Screen with Variable Alphas



Completion of the Calibration Curves

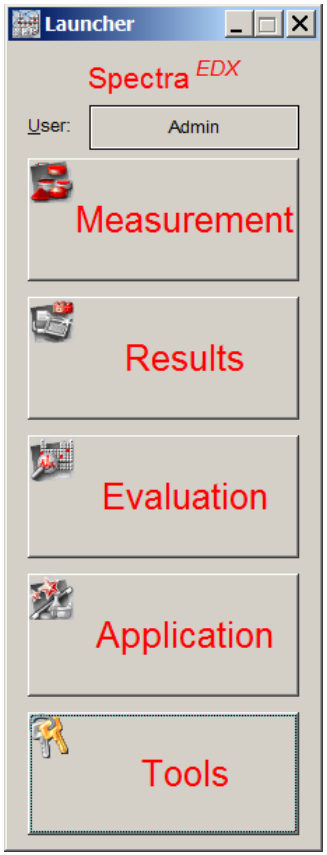
- When all the calibration curves are satisfactory, either click on the Save icon or on the “x” in the top right corner. When the “x” is clicked, a pop-up window will appear asking whether to save the calibration before closing.

- The calibration is saved to a .fcl file with a name chosen by the user. A name based on the material may be suggested, but any name can be used.

- Before using the calibration, an evaluation model must be completed. A .evm file is created with the same name as the .fcl file when the calibration is saved.

5. Selecting Thresholds and transferring cal to the instrument

Opening an evm file



- Click on “Tools”
- Choose “Applications” from the drop-down menu
- Alternatively, the .evm file can be accessed by going to

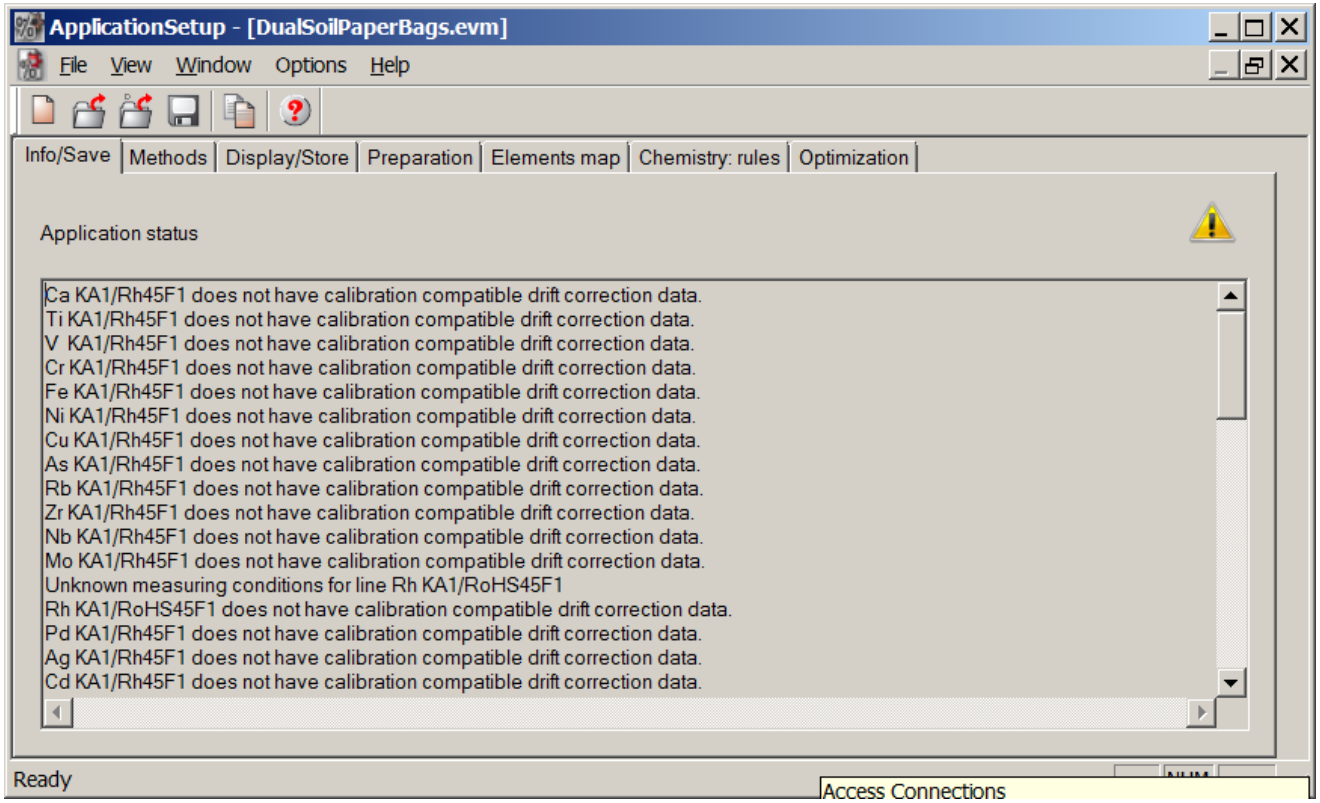
C:\ProgramFiles(x86)\SpectraEDX\ApplicationSetup.exe

Opening an evm file

- Click on “File”, then “Open” from the drop-down menu
- Choose the name of the desired calibration

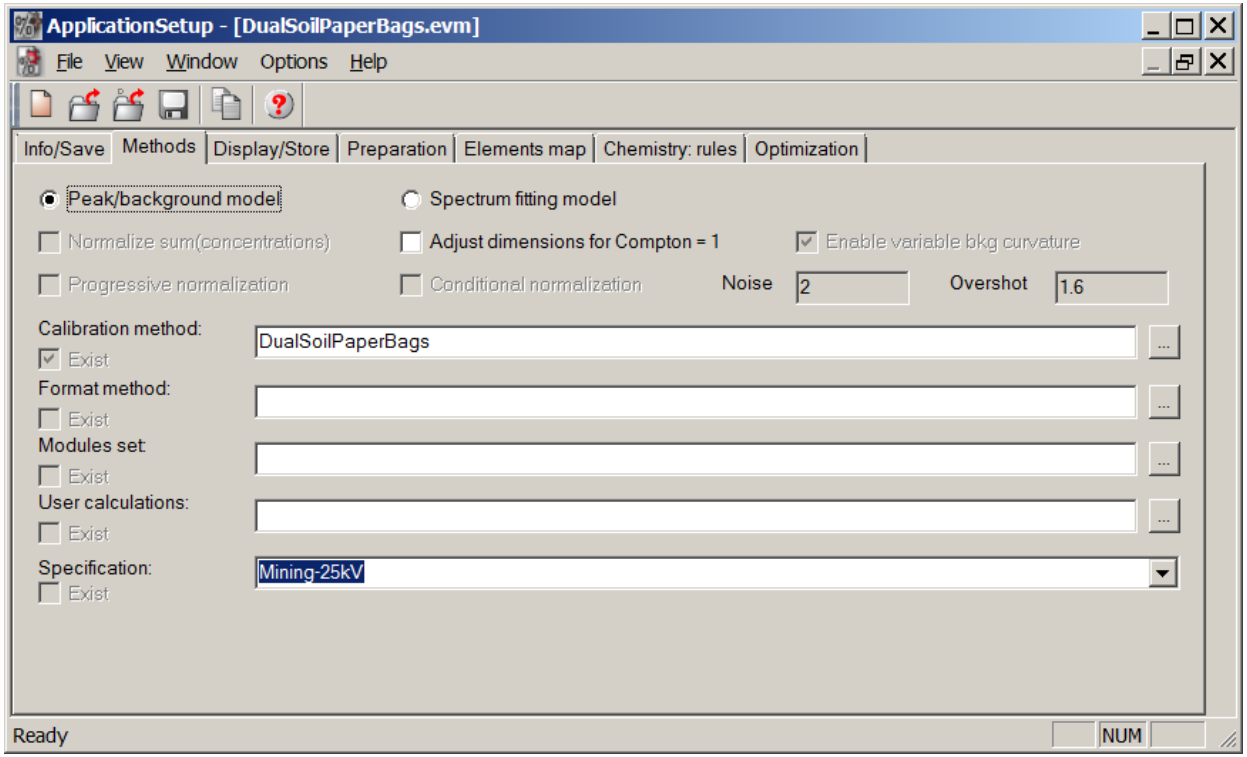
“Save” Screen With Error Reporting

- This screen must be selected in order to save changes
- Errors are reported in the Application Status window
- For handheld (S1) applications, ignore drift correction warnings



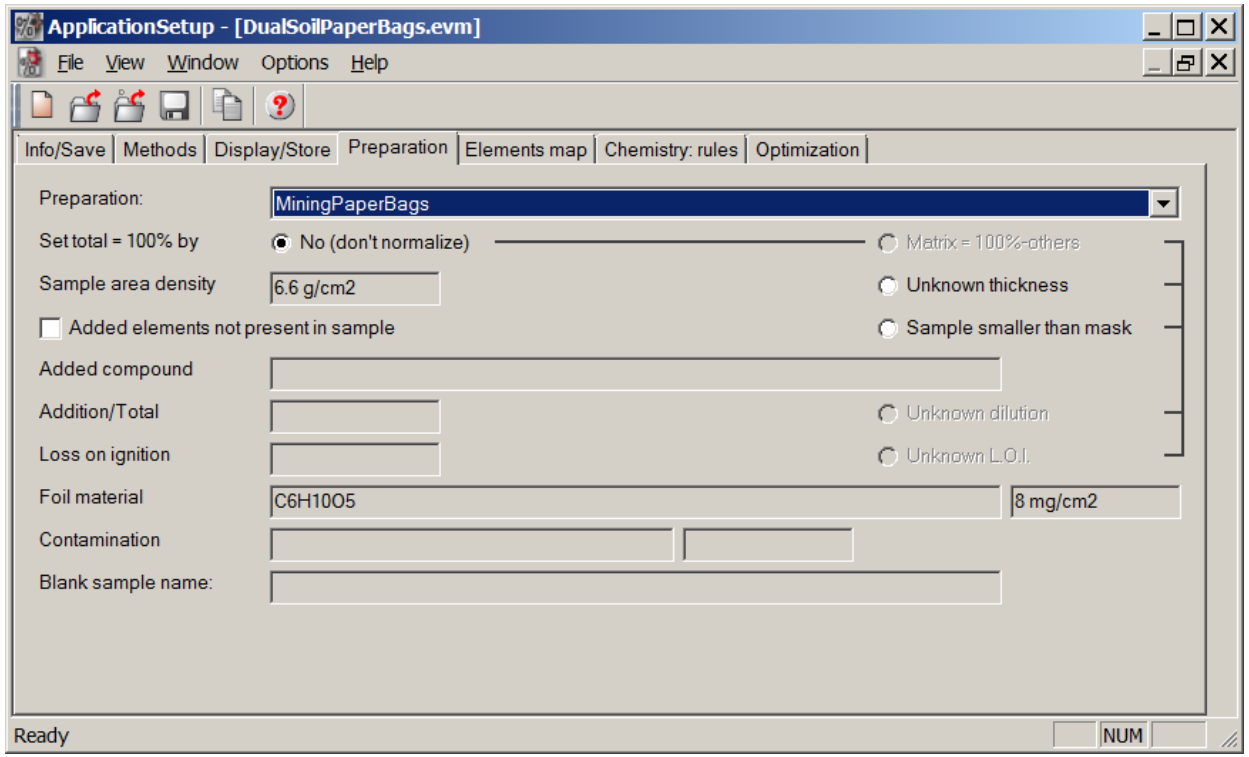
Methods Screen

- Spectrum Fitting and Adjust dimensions are nonfunctional for handheld (S1)
- Normalize sum is available unless a matrix element/compound is chosen
- Progressive and conditional normalization not available for handheld (S1)
- Calibration method = fcl file
- Specification, modules, etc. are not used for handheld (S1)



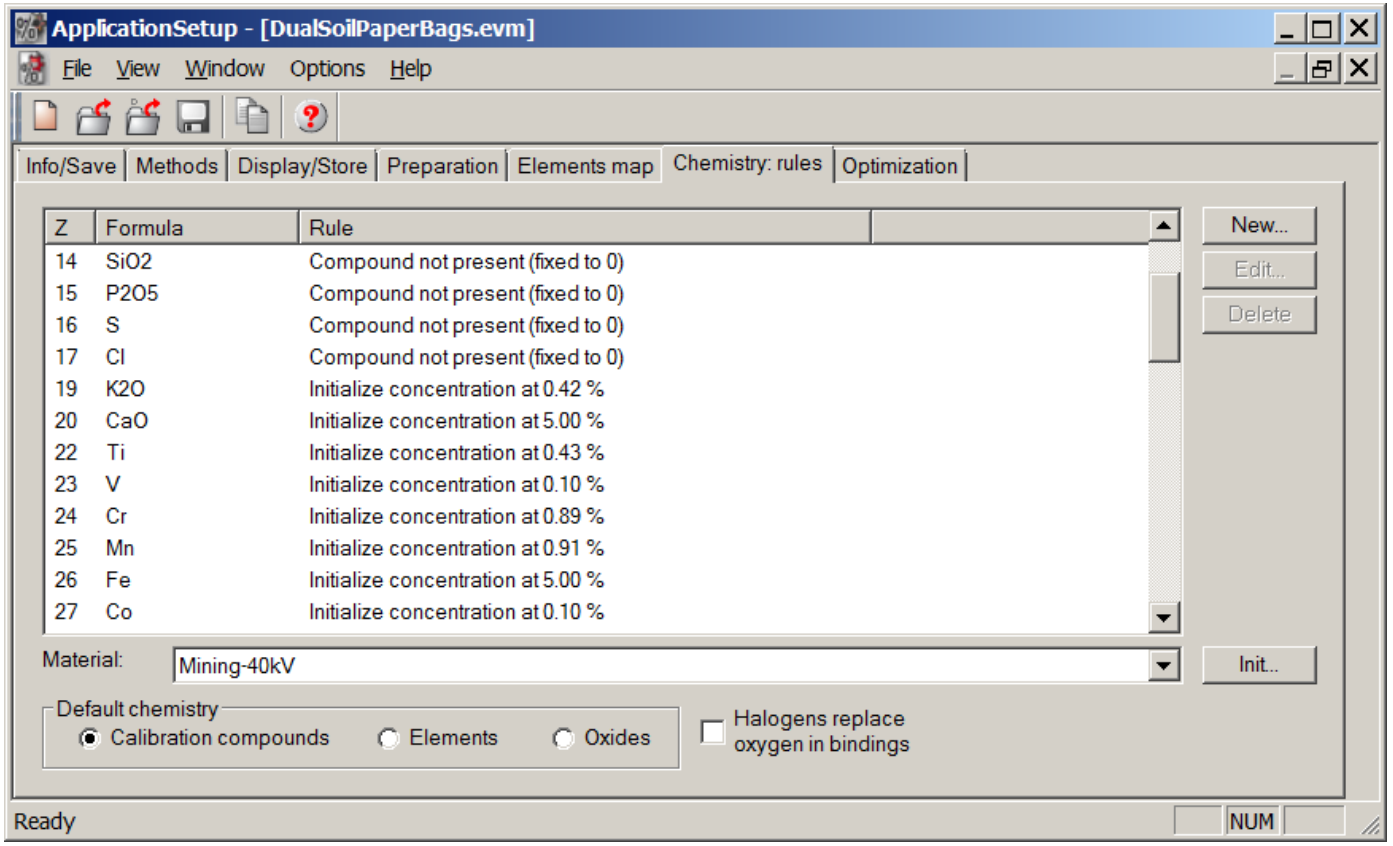
Preparation Screen

- Choose a preparation from the list (created in Application Wizard)
- Preparation must match the unknowns to be measured
- Normalization is not used much in geo applications because of “invisible” elements like C, O, N, etc.

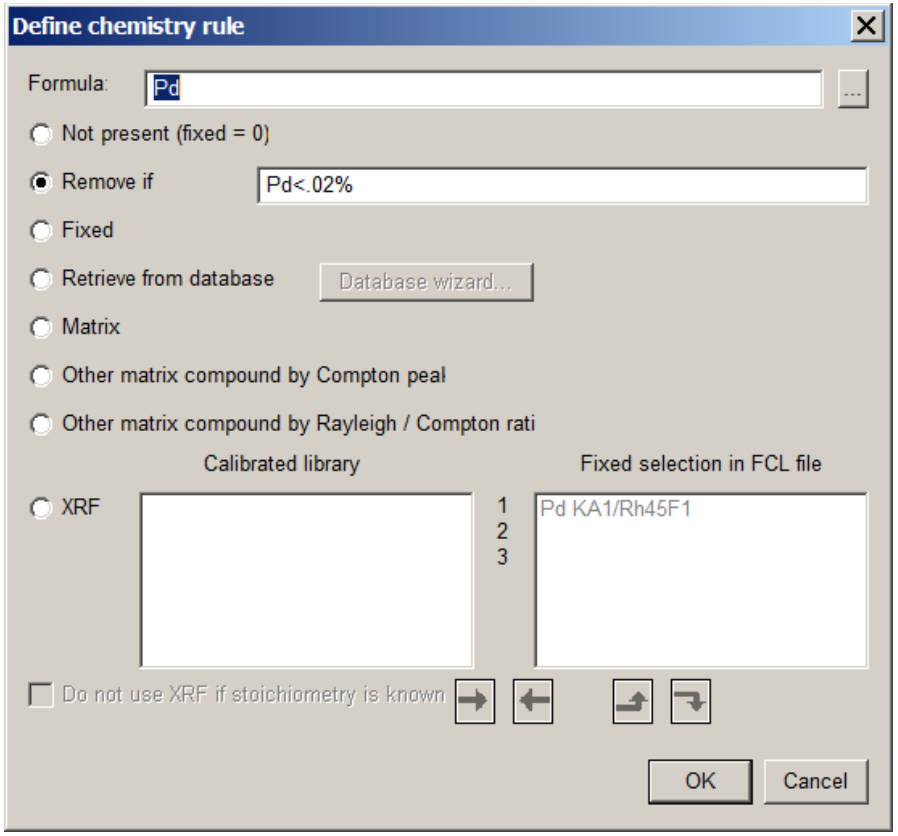


“Chemistry: rules” Screen

- Choose initial concentrations, fix elements to 0, create matrix compounds, add thresholds, determine reporting (oxide vs. element)



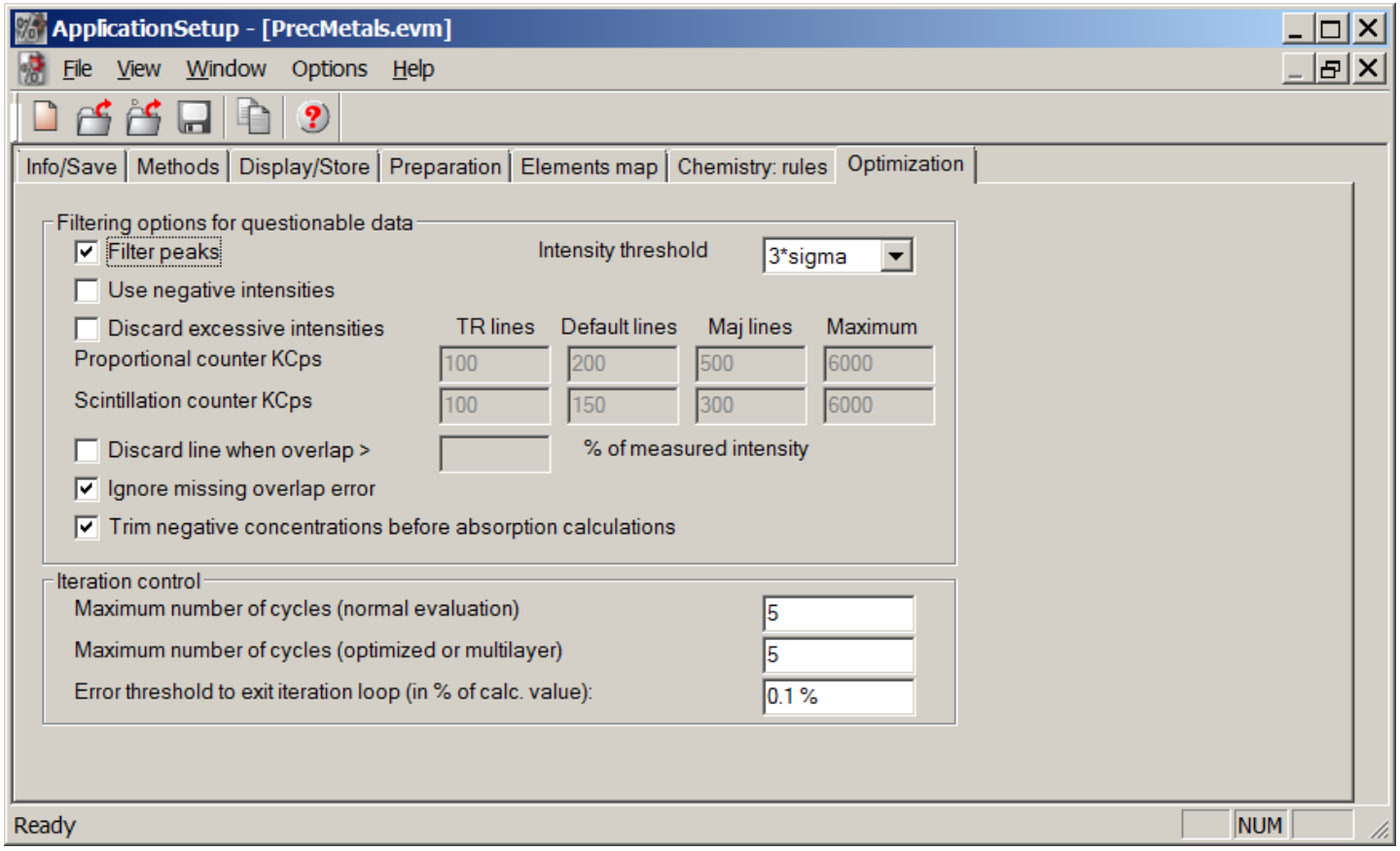
Creating Thresholds



- Use the “Remove if” line to enter thresholds
- Thresholds can be simple, like Pd<.02% or complex, like W>50%&Au<1%
- & is used to indicate complex thresholds
- Multiple thresholds are separated by |
- The presence of large amounts of thresholds will increase calculation time
- This screen (obtained by double clicking on an element) is also used to set as matrix element, not present, or fixed to a single value

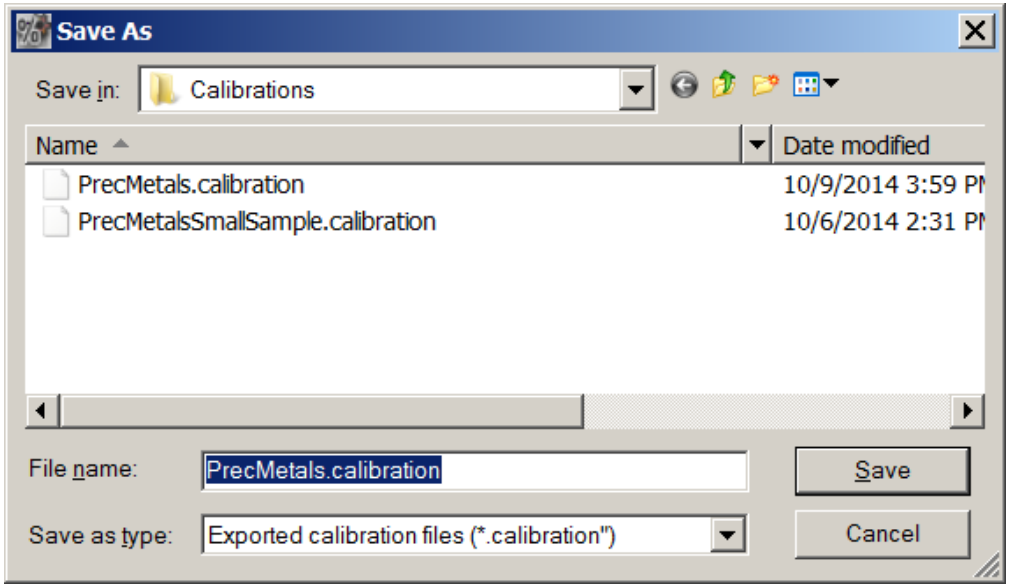
Optimization Screen

- Only the three checked boxes are available for handheld (S1)
- Filter peaks can be used if low concentrations are not needed



Saving as a .calibration File

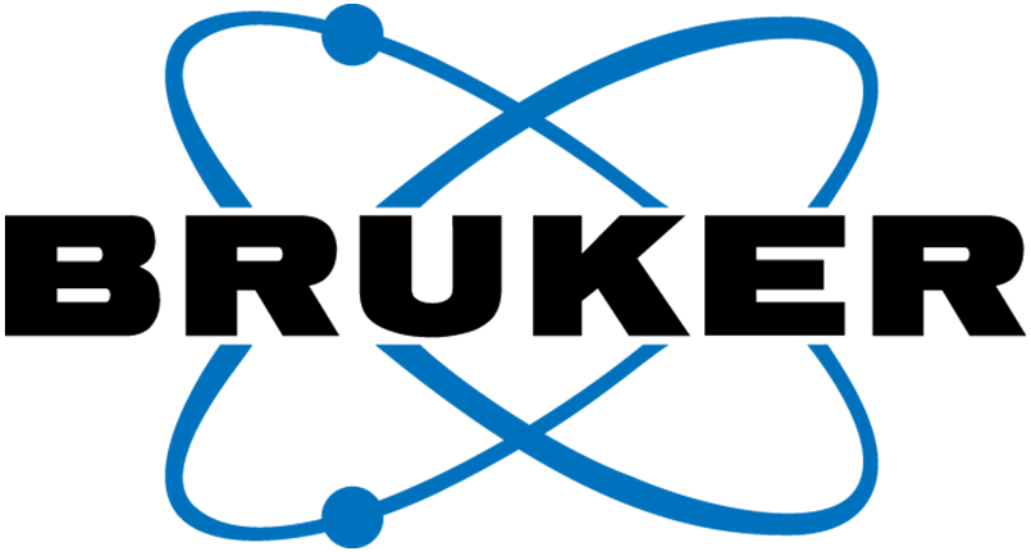
- Click on “File” and choose “Export to calibration file” from the drop-down menu
- The screen below will appear
- Choose an existing file to save over or create a new one by typing in the name at the bottom
- The .calibration file is what is transferred to the instrument



Transferring a Calibration to the Instrument

Files that need to be included and/or modified:

- .calibration
- .aen
- LineLibrary.xrd (if changes were made to the line library)
- LineLibrary.lines (delete if changes were made to the line library)
- .idf (only if new illuminations are used)



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