



# SpectraEDX Training 2014

<b>1</b> <b>H</b> Hydrogen 1.01 0.0007																	<b>2</b> <b>He</b> Helium 4.00 0.0002						
<b>3</b> <b>Li</b> Lithium 6.94 0.53	<b>4</b> <b>Be</b> Beryllium K $\alpha$ 0.108 9.01 1.85																	<b>5</b> <b>B</b> Boron K $\alpha$ 0.183 10.81 2.34	<b>6</b> <b>C</b> Carbon K $\alpha$ 0.277 12.01 2.27	<b>7</b> <b>N</b> Nitrogen K $\alpha$ 0.392 14.01 0.001	<b>8</b> <b>O</b> Oxygen K $\alpha$ 0.525 16.00 0.001	<b>9</b> <b>F</b> Fluorine K $\alpha$ 0.677 19.00 0.001	<b>10</b> <b>Ne</b> Neon K $\alpha$ 0.849 20.18 0.0009
<b>11</b> <b>Na</b> Sodium K $\alpha$ 1.040 22.99 0.97	<b>12</b> <b>Mg</b> Magnesium K $\alpha$ 1.254 24.31 1.74																	<b>13</b> <b>Al</b> Aluminium K $\alpha$ 1.486 26.98 2.70	<b>14</b> <b>Si</b> Silicon K $\alpha$ 1.740 28.09 2.33	<b>15</b> <b>P</b> Phosphorus K $\alpha$ 2.010 30.97 1.82	<b>16</b> <b>S</b> Sulfur K $\alpha$ 2.309 32.07 2.07	<b>17</b> <b>Cl</b> Chlorine K $\alpha$ 2.622 35.45 0.003	<b>18</b> <b>Ar</b> Argon K $\alpha$ 2.958 39.95 0.002
<b>19</b> <b>K</b> Potassium K $\alpha$ 3.314 39.10 0.86	<b>20</b> <b>Ca</b> Calcium K $\alpha$ 3.692 L $\alpha$ 0.341 40.08 1.54	<b>21</b> <b>Sc</b> Scandium K $\alpha$ 4.093 L $\alpha$ 0.395 44.96 2.99	<b>22</b> <b>Ti</b> Titanium K $\alpha$ 4.512 L $\alpha$ 0.452 47.87 4.54	<b>23</b> <b>V</b> Vanadium K $\alpha$ 4.953 L $\alpha$ 0.510 50.94 6.11	<b>24</b> <b>Cr</b> Chromium K $\alpha$ 5.415 L $\alpha$ 0.572 52.00 7.15	<b>25</b> <b>Mn</b> Manganese K $\alpha$ 5.900 L $\alpha$ 0.637 54.94 7.44	<b>26</b> <b>Fe</b> Iron K $\alpha$ 6.405 L $\alpha$ 0.705 55.85 7.87	<b>27</b> <b>Co</b> Cobalt K $\alpha$ 6.931 L $\alpha$ 0.775 58.93 8.86	<b>28</b> <b>Ni</b> Nickel K $\alpha$ 7.480 L $\alpha$ 0.849 58.69 8.91	<b>29</b> <b>Cu</b> Copper K $\alpha$ 8.046 L $\alpha$ 0.928 63.55 8.93	<b>30</b> <b>Zn</b> Zinc K $\alpha$ 8.637 L $\alpha$ 1.012 65.38 7.13	<b>31</b> <b>Ga</b> Gallium K $\alpha$ 9.251 L $\alpha$ 1.098 69.72 5.91	<b>32</b> <b>Ge</b> Germanium K $\alpha$ 9.886 L $\alpha$ 1.188 72.64 5.32	<b>33</b> <b>As</b> Arsenic K $\alpha$ 10.543 L $\alpha$ 1.282 74.92 5.78	<b>34</b> <b>Se</b> Selenium K $\alpha$ 11.224 L $\alpha$ 1.379 78.96 4.81	<b>35</b> <b>Br</b> Bromine K $\alpha$ 11.924 L $\alpha$ 1.481 79.90 3.12	<b>36</b> <b>Kr</b> Krypton K $\alpha$ 12.648 L $\alpha$ 1.585 83.80 0.004						
<b>37</b> <b>Rb</b> Rubidium K $\alpha$ 13.396 L $\alpha$ 1.692 85.47 1.53	<b>38</b> <b>Sr</b> Strontium K $\alpha$ 14.165 L $\alpha$ 1.806 87.62 2.64	<b>39</b> <b>Y</b> Yttrium K $\alpha$ 14.958 L $\alpha$ 1.924 88.91 4.47	<b>40</b> <b>Zr</b> Zirconium K $\alpha$ 15.775 L $\alpha$ 2.044 91.22 6.51	<b>41</b> <b>Nb</b> Niobium K $\alpha$ 16.615 L $\alpha$ 2.169 92.91 8.57	<b>42</b> <b>Mo</b> Molybdenum K $\alpha$ 17.480 L $\alpha$ 2.292 95.94 10.22	<b>43</b> <b>Tc</b> Technetium K $\alpha$ 18.367 L $\alpha$ 2.423 (98) 11.50	<b>44</b> <b>Ru</b> Ruthenium K $\alpha$ 19.279 L $\alpha$ 2.558 101.07 12.37	<b>45</b> <b>Rh</b> Rhodium K $\alpha$ 20.216 L $\alpha$ 2.697 102.91 12.41	<b>46</b> <b>Pd</b> Palladium K $\alpha$ 21.177 L $\alpha$ 2.838 106.42 12.02	<b>47</b> <b>Ag</b> Silver K $\alpha$ 22.163 L $\alpha$ 2.983 107.87 10.50	<b>48</b> <b>Cd</b> Cadmium K $\alpha$ 23.173 L $\alpha$ 3.133 112.41 8.69	<b>49</b> <b>In</b> Indium K $\alpha$ 24.210 L $\alpha$ 3.286 114.82 7.31	<b>50</b> <b>Sn</b> Tin K $\alpha$ 25.271 L $\alpha$ 3.444 118.71 7.29	<b>51</b> <b>Sb</b> Antimony K $\alpha$ 26.359 L $\alpha$ 3.604 121.76 6.69	<b>52</b> <b>Te</b> Tellurium K $\alpha$ 27.473 L $\alpha$ 3.768 127.60 6.23	<b>53</b> <b>I</b> Iodine K $\alpha$ 28.612 L $\alpha$ 3.938 126.90 4.93	<b>54</b> <b>Xe</b> Xenon K $\alpha$ 29.775 L $\alpha$ 4.110 131.29 0.006						
<b>55</b> <b>Cs</b> Cesium K $\alpha$ 30.973 L $\alpha$ 4.285 132.91 1.87	<b>56</b> <b>Ba</b> Barium K $\alpha$ 32.194 L $\alpha$ 4.466 137.33 3.59	<b>57</b> <b>La</b> Lanthanum K $\alpha$ 33.442 L $\alpha$ 4.647 138.91 6.15	<b>72</b> <b>Hf</b> Hafnium K $\alpha$ 7.899 M $\alpha$ 1.646 178.49 13.31	<b>73</b> <b>Ta</b> Tantalum K $\alpha$ 8.146 M $\alpha$ 1.712 180.95 16.65	<b>74</b> <b>W</b> Tungsten K $\alpha$ 8.398 M $\alpha$ 1.775 183.84 19.25	<b>75</b> <b>Re</b> Rhenium K $\alpha$ 8.652 M $\alpha$ 1.843 186.21 21.02	<b>76</b> <b>Os</b> Osmium K $\alpha$ 8.911 M $\alpha$ 1.907 190.23 22.61	<b>77</b> <b>Ir</b> Iridium K $\alpha$ 9.175 M $\alpha$ 1.980 192.22 22.65	<b>78</b> <b>Pt</b> Platinum K $\alpha$ 9.442 M $\alpha$ 2.050 195.08 21.46	<b>79</b> <b>Au</b> Gold K $\alpha$ 9.713 M $\alpha$ 2.123 196.97 19.28	<b>80</b> <b>Hg</b> Mercury K $\alpha$ 9.989 M $\alpha$ 2.195 200.59 13.53	<b>81</b> <b>Tl</b> Thallium K $\alpha$ 10.269 M $\alpha$ 2.271 204.37 11.85	<b>82</b> <b>Pb</b> Lead K $\alpha$ 10.551 M $\alpha$ 2.342 207.20 11.34	<b>83</b> <b>Bi</b> Bismuth K $\alpha$ 10.839 M $\alpha$ 2.423 208.98 9.81	<b>84</b> <b>Po</b> Polonium K $\alpha$ 11.131 M $\alpha$ 2.499 (209) 9.32	<b>85</b> <b>At</b> Astatine K $\alpha$ 11.427 M $\alpha$ 2.577 (210) 7.00	<b>86</b> <b>Rn</b> Radon K $\alpha$ 11.727 M $\alpha$ 2.654 (222) 0.01						
<b>87</b> <b>Fr</b> Francium K $\alpha$ 12.031 M $\alpha$ 2.732 (223) 1.87	<b>88</b> <b>Ra</b> Radium K $\alpha$ 12.339 M $\alpha$ 2.806 (226) 5.50	<b>89</b> <b>Ac</b> Actinium K $\alpha$ 12.652 M $\alpha$ 2.900 (227) 10.07																					
<b>58</b> <b>Ce</b> Cerium K $\alpha$ 4.839 M $\alpha$ 0.884 140.12 6.77	<b>59</b> <b>Pr</b> Praseodymium K $\alpha$ 5.035 M $\alpha$ 0.927 140.91 6.77	<b>60</b> <b>Nd</b> Neodymium K $\alpha$ 5.228 M $\alpha$ 0.979 144.24 7.01	<b>61</b> <b>Pm</b> Promethium K $\alpha$ 5.432 M $\alpha$ 1.023 (145) 7.26	<b>62</b> <b>Sm</b> Samarium K $\alpha$ 5.633 M $\alpha$ 1.078 150.36 7.52	<b>63</b> <b>Eu</b> Europium K $\alpha$ 5.849 M $\alpha$ 1.131 151.96 5.24	<b>64</b> <b>Gd</b> Gadolinium K $\alpha$ 6.053 M $\alpha$ 1.181 157.25 7.90	<b>65</b> <b>Tb</b> Terbium K $\alpha$ 6.273 M $\alpha$ 1.240 158.93 8.23	<b>66</b> <b>Dy</b> Dysprosium K $\alpha$ 6.498 M $\alpha$ 1.293 162.50 8.55	<b>67</b> <b>Ho</b> Holmium K $\alpha$ 6.720 M $\alpha$ 1.348 164.93 8.80	<b>68</b> <b>Er</b> Erbium K $\alpha$ 6.949 M $\alpha$ 1.404 167.26 9.07	<b>69</b> <b>Tm</b> Thulium K $\alpha$ 7.180 M $\alpha$ 1.462 168.93 9.32	<b>70</b> <b>Yb</b> Ytterbium K $\alpha$ 7.416 M $\alpha$ 1.526 173.04 6.97	<b>71</b> <b>Lu</b> Lutetium K $\alpha$ 7.655 M $\alpha$ 1.580 174.47 9.84										
<b>90</b> <b>Th</b> Thorium K $\alpha$ 11.72 L $\alpha$ 1.481 232.04 11.72	<b>91</b> <b>Pa</b> Protactinium K $\alpha$ 15.37 L $\alpha$ 1.999 231.04 15.37	<b>92</b> <b>U</b> Uranium K $\alpha$ 18.95 L $\alpha$ 2.044 238.03 18.95	<b>93</b> <b>Np</b> Neptunium K $\alpha$ 20.45 L $\alpha$ 2.144 (237) 20.45	<b>94</b> <b>Pu</b> Plutonium K $\alpha$ 19.84 L $\alpha$ 2.199 (244) 19.84	<b>95</b> <b>Am</b> Americium K $\alpha$ 13.69 L $\alpha$ 2.286 (243) 13.69	<b>96</b> <b>Cm</b> Curium K $\alpha$ 13.51 L $\alpha$ 2.344 (247) 13.51	<b>97</b> <b>Bk</b> Berkelium K $\alpha$ 14.79 L $\alpha$ 2.402 (247) 14.79	<b>98</b> <b>Cf</b> Californium K $\alpha$ 15.1 L $\alpha$ 2.459 (251) 15.1	<b>99</b> <b>Es</b> Einsteinium K $\alpha$ 13.5 L $\alpha$ 2.517 (252) 13.5	<b>100</b> <b>Fm</b> Fermium K $\alpha$ 14.04 L $\alpha$ 2.574 (257) 14.04	<b>101</b> <b>Md</b> Mendelevium K $\alpha$ 14.62 L $\alpha$ 2.631 (258) 14.62	<b>102</b> <b>No</b> Nobelium K $\alpha$ 15.26 L $\alpha$ 2.688 (259) 15.26	<b>103</b> <b>Lr</b> Lawrencium K $\alpha$ 15.80 L $\alpha$ 2.745 (262) 15.80										



Atomic number

Atomic weight

Density (g/cm<sup>3</sup>)

Symbol

Element name

Energy (keV)

**35** 79.90  
**Br** 3.12  
Bromine  
K $\alpha$  11.924  
L $\alpha$  1.481

# 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



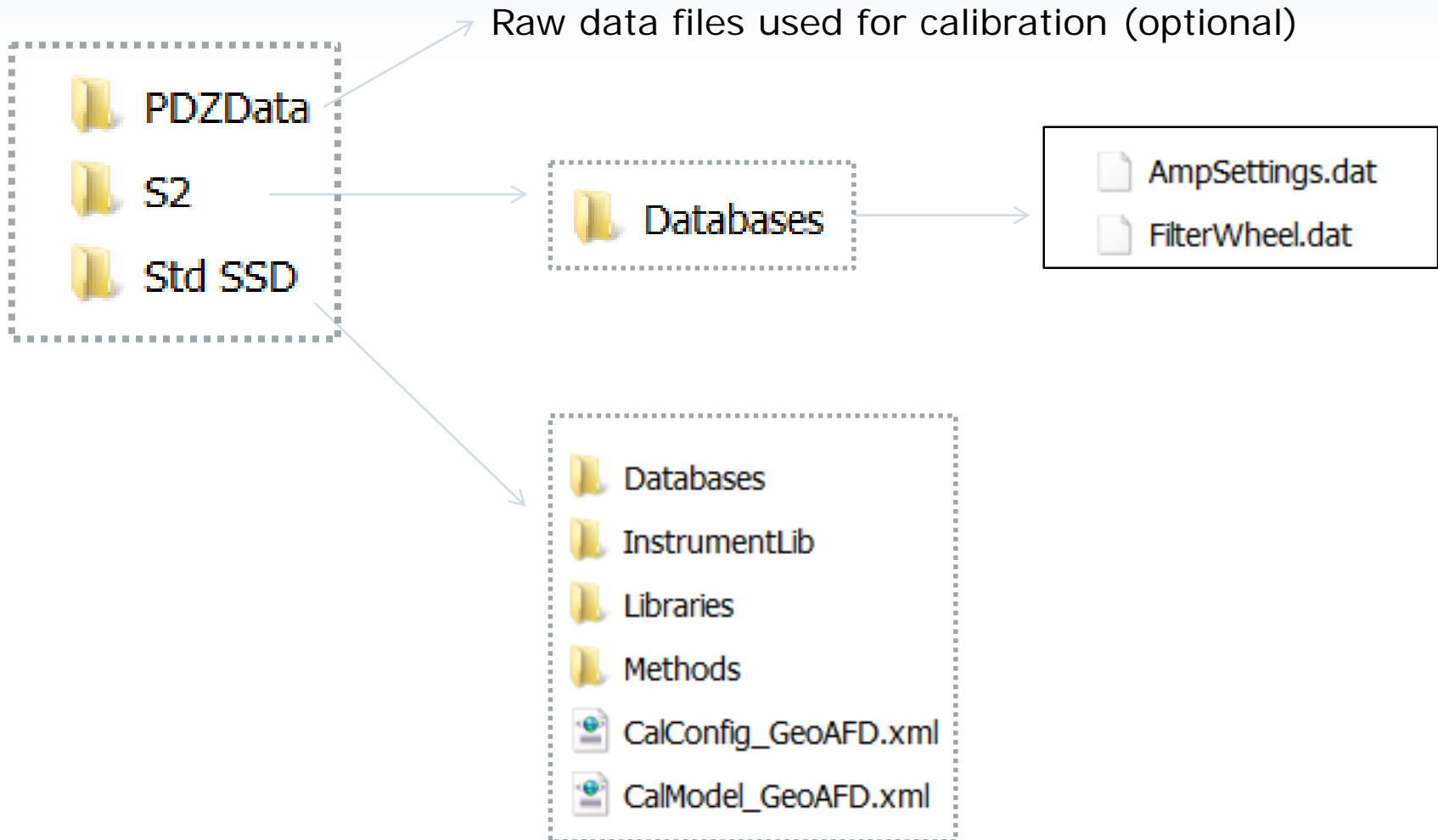
SpectraEDX was designed for use on a computer connected to a single S2 Ranger or other benchtop unit

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.

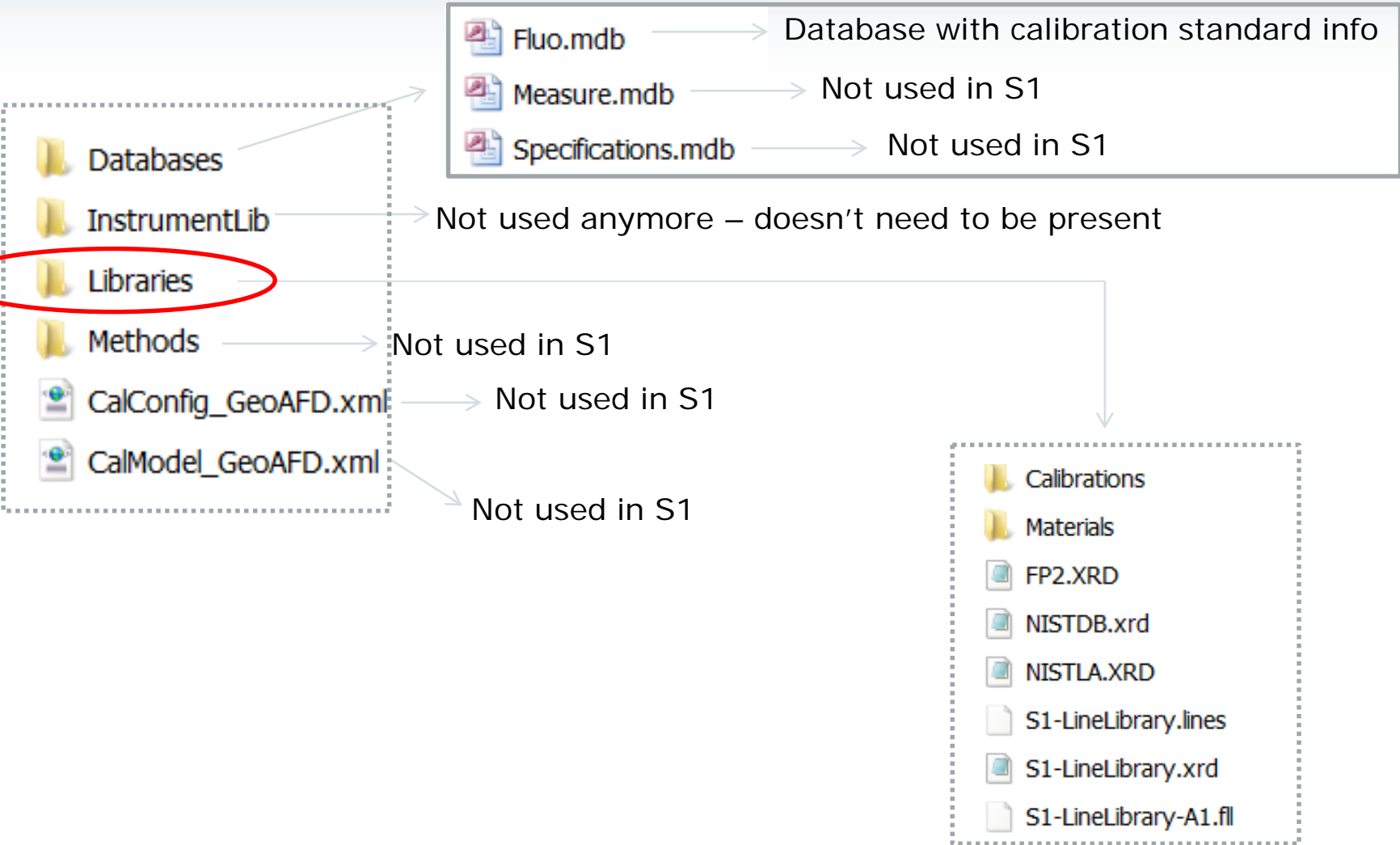
Having multiple SpectraEDX calibration files on one computer requires the use of multiple pointer files or a substitution (S:\) drive.

# 1. File Structure of SpectraEDX

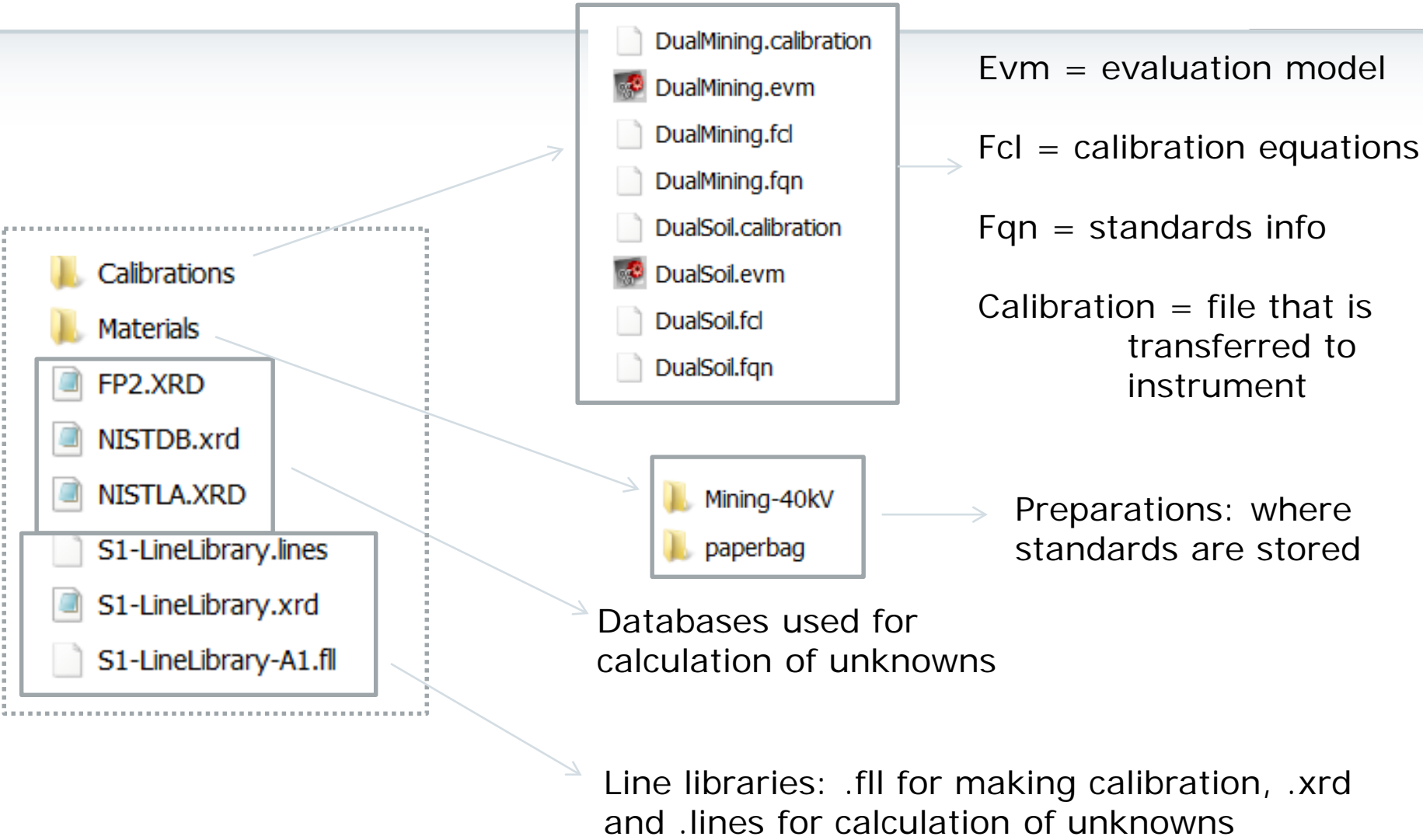
# File Structure (part 1) – Top Level Folder



# File Structure (part 2) – Mid Level Folders



# File Structure (part 3) - Libraries



## 2. Setting up the Calibration Standards

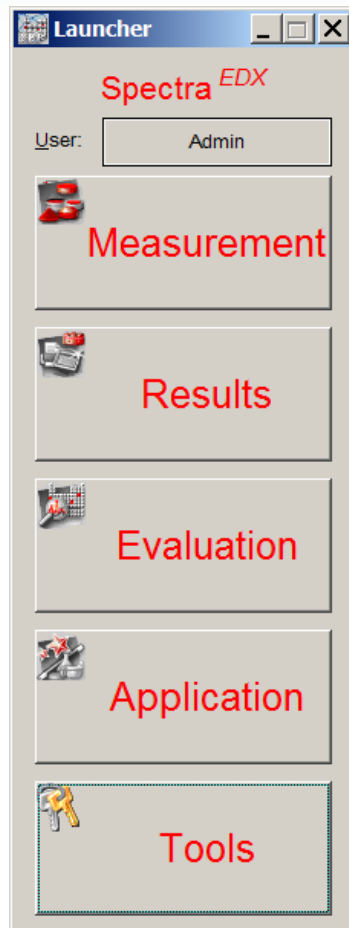


# Basic Steps for Defining Calibration Standards



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)

The screenshot shows the "ApplicationWizard" software window. The title bar reads "ApplicationWizard - [DualSoil.evm]". The menu bar includes "File", "Edit", "View", "Method", "Calibration", "Window", "Options", and "Help". The toolbar contains various icons for file operations and navigation. On the left, a tree view shows a hierarchy of folders: "DualSoil", "Materials", "Preparation", "Prepared Standards", "Measurement", "Calibration", "Modules", "Limits Check", "Results Formatting", "Application", and "S2 Ranger Application". The main content area displays the "ApplicationWizard Program" instructions. At the top of the main area, it says "Please push 'Next' button". The instructions include:

**ApplicationWizard Program**  
ApplicationWizard makes it possible to define an XRF Application by a succession of automated 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).

**Opening a Spectra<sup>EDX</sup> Application file:**  
Use the File | Open command to open an Application (EVM file), or a Draft Application (DEVM file). The Application files were formerly referred to as Evaluation Models in Spectra<sup>EDX</sup> version 2.2 and below, but are now referred to as Application files. Draft Applications are unfinished Applications, these will be converted to finished Applications (EVM) at the second to 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 next to last step (the Application step).

**Making another application** (e.g. with different corrections) from the same data:

1. Create an empty document, giving it a name.
2. Review the steps down to the **Calibration** step making the same selections as before.
3. Define the new calibration at the Calibration step.
4. Then proceed as usual.

**Defining a new preparation:**

1. Go to the Setup mode (use the pliers tool or the File Setup mode menu)
2. Go to the **Preparation | Parameters** step,
3. Enter the new preparation name. The new preparation will be a copy of the currently selected preparation.
4. Make needed changes on the **Parameters, Size, Contamination, and Foil** screens
5. The changes to the database are automatically saved.

**Defining a new compound** (which will be available in the **Materials | Compounds** step):

# Calibration "Tree" List



Expanded

# Materials Page – choose material group and material



ApplicationWizard - [DualSoil.levm]

File Edit View Method Calibration Window Options Help

Material groups: Mining

Materials:  
New material:

Name	Elem...	Standa...	Date of creation	Date of last chang...
Mining-25kV	0	0	29-Dec-2009 10:10...	29-Dec-2009 10:1...
Mining-40kV	50	222	30-Mar-2009 22:27...	01-May-2012 14:3...

List of materials for the current material group.

Status NUM

# 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



ApplicationWizard - [DualSoil.ewm]

File Edit View Method Calibration Window Options Help

Material group: **Mining** Material: **Mining-40kV**

Compound list:

Name ...	Form...	Z	Or...	Spe...
Sodi...	Na2O	11	1	
Magn...	Mg	12	2	
Alumin...	Al	13	3	
Silicon	Si	14	4	
Phosp...	P	15	5	
Sulfur	S	16	6	
Potas...	K	19	7	
Calcium	Ca	20	8	
Titanium	Ti	22	9	
Vanad...	V	23	10	
Chrom...	Cr	24	11	
Mang...	Mn	25	12	
Iron	Fe	26	13	
Cobalt	Co	27	14	
Nickel	Ni	28	15	
Copper	Cu	29	16	
Zinc	Zn	30	17	
Arsenic	As	33	18	
Seleni...	Se	34	19	
Rubidi...	Rb	37	20	
Stronti...	Sr	38	21	
Zirconi...	Zr	40	22	
Niobium	Nb	41	23	
Molyb...	Mo	42	24	
Rhodium	Rh	45	25	
Pallad...	Pd	46	26	
Silver	Ag	47	27	
Cadmi...	Cd	48	28	
Tin	Sn	50	29	
Antimo...	Sb	51	30	
Cerium	Ce	58	31	
Uranium	U	92	32	

For Help, press F1

Status NUM



# Choosing Compounds in the Material



ApplicationWizard - [DualSoil.evm]

File Edit View Method Calibration Window Options Help

Material group: **Minine** Material: **Minine-40kV**

All compounds:

Name	Formula	Z
Wax	CH2	6
Water	H2O	1
Tungsten Carbide	WC	74
Polypropylene	CH2	6
Oil	CH2	6
Mylar	C10H8O4	6
Mn3O4	Mn3O4	25
Manganese(IV)Oxide	MnO2	25
Manganese(II,IV)Oxide	Mn2O3	25
Lithiumtetraborate	Li2B4O7	3
Lithiummetaborate	LiBO2	5
Lithiumbromide	LiBr	35
LOI	CO2	6
Ironsulfide	FeS	16
Iron-II-oxid	FeO	26
Iron-(II,III)-oxide	Fe3O4	26
HCl	HCl	17
H2O	H2O	1
Cordierite	2MgO,2Al2O3,5SiO2	14
Cobalt II-III oxide	Co3O4	27
Cellulose	C6H10O5	8
Carbon dioxide	CO2	6
Calciumcarbonate	CaCO3	20
Calcium fluoride	CaF2	20
CO2	CO2	6
CH2	CH2	6
Boric Acid	H3BO3	5

Compound list:

Name ...	Form...	Z	Or... \	Spe...
Sodiu...	Na2O	11	1	
Magn...	Mg	12	2	
Alumin...	Al	13	3	
Silicon	Si	14	4	
Phosp...	P	15	5	
Sulfur	S	16	6	
Potas...	K	19	7	
Calcium	Ca	20	8	
Titanium	Ti	22	9	
Vanad...	V	23	10	
Chrom...	Cr	24	11	
Mang...	Mn	25	12	
Iron	Fe	26	13	
Cobalt	Co	27	14	
Nickel	Ni	28	15	
Copper	Cu	29	16	
Zinc	Zn	30	17	
Arsenic	As	33	18	
Seleni...	Se	34	19	
Rubidi...	Rb	37	20	
Stronti...	Sr	38	21	
Zirconi...	Zr	40	22	
Niobium	Nb	41	23	
Molyb...	Mo	42	24	
Rhodium	Rh	45	25	
Pallad...	Pd	46	26	
Silver	Ag	47	27	
Cadmi...	Cd	48	28	
Tin	Sn	50	29	
Antimo...	Sb	51	30	
Cerium	Ce	58	31	
U...	U	92	92	

DualSoil... For Help, press F1 Status NUM

# Inputting Names and Data for Standards



ApplicationWizard - [DualSoil.levm]

File Edit View Method Calibration Window Options Help

Material group: Mining Material: Mining-40kV

Limits: 95.0 105.0 %  (Auto) New standard

Display concentrations per:  Compounds  Elements After validation, go to:  Bottom  Right

	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	1.400	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	1.400	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
M4515AMIS063	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
Mining-40kV															

Automatic Unit:  PPM  %

Type "B" for Balance, "T" for Trace or use contextual menu.

Print Paste with Titles

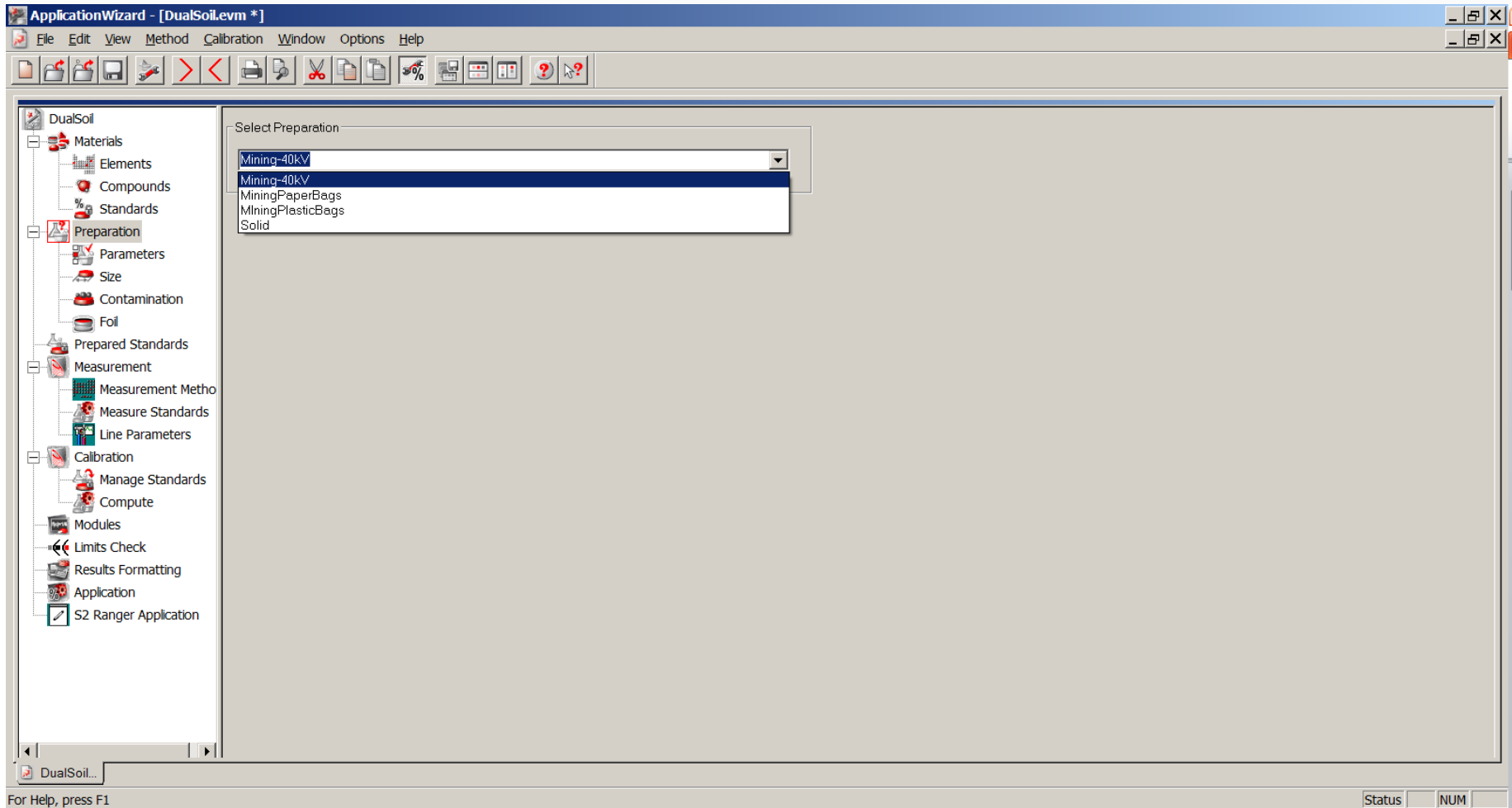
DualSoil... For Help, press F1 Status NUM

# 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



The screenshot shows the 'ApplicationWizard' software interface for 'DualSoil'. The window title is 'ApplicationWizard - [DualSoil.levm \*]'. The menu bar includes 'File', 'Edit', 'View', 'Method', 'Calibration', 'Window', 'Options', and 'Help'. The toolbar contains various icons for file operations and navigation.

The left sidebar shows a tree view of the software's structure:

- DualSoil
  - Materials
    - Elements
    - Compounds
    - Standards
  - Preparation
    - Parameters
    - Size
    - Contamination
    - Foil
    - Prepared Standards
  - Measurement
    - Measurement Method
    - Measure Standards
    - Line Parameters
  - Calibration
    - Manage Standards
    - Compute
  - Modules
  - Limits Check
  - Results Formatting
  - Application
    - S2 Ranger Application

The main workspace is titled 'Preparation' and contains the following fields and controls:

- Preparation:** A dropdown menu showing 'MiningPaperBags' with a close button (X).
- New preparation:** An empty text input field with a file icon.
- Method:** A dropdown menu with 'Loose Powder' selected. The list includes: Solid, Fused Bead, Pressed Pellet, Loose Powder, Liquid, Solution, and Tablet.
- Addition:** A list with a '+' sign and a checkbox. The selected item is 'Loose Powder'.
- Material + Additive:** A row with a checkbox, a text input field containing '100.', the unit 'g', and a percentage sign '%'. Below this is the label 'Material + Additive'.
- Ratio:** A section with two rows of input fields:
  - Row 1: 'Original material' = 1, 'Total' = 1.
  - Row 2: 'Original material' = 1, 'Binder/flux' = 0.
- Dilution:** A section with two rows of input fields:
  - Row 1: 'Original material/Total' = 1.
  - Row 2: 'Original material/Additive' = 0.
  - Checkbox: 'Unknown dilution'.

The status bar at the bottom left says 'For Help, press F1'. The status bar at the bottom right shows 'Status' and 'NUM'.

# Infinite Thickness Calculation



ApplicationWizard - [DualSoil.evm \*]

File Edit View Method Calibration Window Options Help

DualSoil

- Materials
  - Elements
  - Compounds
  - Standards
- Preparation
  - Parameters
  - Size
- Contamination
- Foil
- Prepared Standards
- Measurement
  - Measurement Method
  - Measure Standards
  - Line Parameters
- Calibration
  - Manage Standards
  - Compute
- Modules
- Limits Check
- Results Formatting
- Application
- S2 Ranger Application

Preparation: MiningPaperBags

Size

Area density: 6.6 g/cm<sup>2</sup>

Area: 12.5664 cm<sup>2</sup>

Mass: 100. g

Diameter: 4. cm

Mass: 100. g

Thickness: 2.2 cm

Density: 3. g/cm<sup>3</sup>

Diameter Thickness Density

Diameter Thickness Mass

Diameter Mass Density

For Help, press F1

Status NUM

# "Foil" Attenuation Definition



The screenshot shows the 'ApplicationWizard' software interface for 'DualSoil.levm'. The 'Preparation' dropdown is set to 'MiningPaperBags'. The 'Foil material' dropdown is set to 'paperbag'. The 'Area density' is set to  $8.8 \times 10^{-3}$  g/cm<sup>2</sup>. The 'Area' is set to cm<sup>2</sup> and 'Mass' is set to g. The 'Diameter' is set to cm and 'Mass' is set to g. The 'Thickness' is set to 100 μm and 'Density' is set to 0.8 g/cm<sup>3</sup>. The 'Foil' option is selected in the 'Preparation' section of the left-hand tree view.

ApplicationWizard - [DualSoil.levm \*]  
File Edit View Method Calibration Window Options Help

Preparation: MiningPaperBags

Foil material: paperbag

Area density:  $8.8 \times 10^{-3}$  g/cm<sup>2</sup>

Area: cm<sup>2</sup> Mass: g

Diameter: cm Mass: g

Thickness: 100 μm Density: 0.8 g/cm<sup>3</sup>

For Help, press F1

Status NUM

# Choosing the Prepared Standards



ApplicationWizard - [DualSoil.levm \*]

File Edit View Method Calibration Window Options Help

Material group: Mining Material: Mining-40kV Preparation: MiningPaperBags

Standard Material: M45WO3 New Prepared Standard: M45WO3

Automatically create all prepared standards  Short names

Display prepared standards  All standard materials  All preparations

Std. Material	Preparation	Prep. Standard	Thickness (cm)	Density (g/cm3)
<input checked="" type="checkbox"/> Field-054	MiningPaperBags	Field-054	2.20	3.000
<input checked="" type="checkbox"/> Field-065	MiningPaperBags	Field-065	2.20	3.000
<input checked="" type="checkbox"/> Field-266	MiningPaperBags	Field-266	2.20	3.000
<input checked="" type="checkbox"/> Field-394	MiningPaperBags	Field-394	2.20	3.000
<input checked="" type="checkbox"/> Field-523	MiningPaperBags	Field-523	2.20	3.000
<input checked="" type="checkbox"/> Field-528	MiningPaperBags	Field-528	2.20	3.000
<input checked="" type="checkbox"/> Field-816	MiningPaperBags	Field-816	2.20	3.000
<input checked="" type="checkbox"/> Field-822	MiningPaperBags	Field-822	2.20	3.000
<input checked="" type="checkbox"/> M4515AGV_2	Mining-40kV	M4515AGV_2	2.20	3.000
<input checked="" type="checkbox"/> M4515AK396	Mining-40kV	M4515AK396	2.20	3.000
<input checked="" type="checkbox"/> M4515AK397	Mining-40kV	M4515AK397	2.20	3.000
<input checked="" type="checkbox"/> M4515AK401	Mining-40kV	M4515AK401	2.20	3.000
<input checked="" type="checkbox"/> M4515AK402	Mining-40kV	M4515AK402	2.20	3.000
<input checked="" type="checkbox"/> M4515AK408	Mining-40kV	M4515AK408	2.20	3.000
<input checked="" type="checkbox"/> M4515AK411	Mining-40kV	M4515AK411	2.20	3.000
<input checked="" type="checkbox"/> M4515AK423	Mining-40kV	M4515AK423	2.20	3.000
<input checked="" type="checkbox"/> M4515AK426	Mining-40kV	M4515AK426	2.20	3.000
<input checked="" type="checkbox"/> M4515AMIS008	Mining-40kV	M4515AMIS008	2.20	3.000
<input checked="" type="checkbox"/> M4515AMIS013	Mining-40kV	M4515AMIS013	2.20	3.000
<input checked="" type="checkbox"/> M4515AMIS014	Mining-40kV	M4515AMIS014	2.20	3.000
<input checked="" type="checkbox"/> M4515AMIS015	Mining-40kV	M4515AMIS015	2.20	3.000
<input checked="" type="checkbox"/> M4515AMIS022	Mining-40kV	M4515AMIS022	2.20	3.000
<input checked="" type="checkbox"/> M4515AMIS027	Mining-40kV	M4515AMIS027	2.20	3.000

DualSoil...

The definition of the material has been changed at this step; do you want to save the changes? Status NUM



### 3. Using and editing the Line Library

# Line Library Access #1



## Launcher: Tools → Line Library Maintenance

LibManager V2.2.75

System:  WDX  EDX

Display:  Default Library  Special Library

Path: S:\Std SSD\Libraries\S1-LineLibrary-A1.fil

Text format

Toggle Select lines from methods

Show selected lines first  Show drift correction details  Show calibration details

Copy selection to clipboard

1 out of 209 lines selected. Sort Z

Z	Line N...	Comment	line keV	tube KV	Filter	Ref Sample	Ref Line	Calib.	Intensity	Detector
8	O KA1	VerA1F	0.5249	5					Integr.	Normal
12	Mg KA1	AL15	1.253	15					Integr.	Normal
12	Mg KA1	Alloy15	1.253	15					Integr.	Normal
12	Mg KA1	Mine15	1.253	15					Integr.	Normal
13	Al KA1	AL15	1.487	15		TM15AL6061TA	Al KA1/AL15		Integr.	Normal
13	Al KA1	AL25	1.487	25					Integr.	Normal
13	Al KA1	Alloy15	1.487	15		TM15AL6061TA	Al KA1/Alloy15		Integr.	Normal
14	Si KA1	AL15	1.74	15					Integr.	Normal
14	Si KA1	Alloy15	1.74	15					Integr.	Normal
14	Si KA1	Mine15	1.74	15					Integr.	Normal
14	Si KA1	Mine40	1.74	40	Ti 25um...				Integr.	Normal
15	P KA1	Alloy15	2.014	15					Integr.	Normal
15	P KA1	Mine15	2.014	15					Integr.	Normal
16	S KA1	Alloy15	2.308	15					Integr.	Normal
16	S KA1	Mine15	2.308	15					Integr.	Normal
17	Cl KA1	Alloy15	2.622	15					Integr.	Normal
17	Cl KA1	Mine15	2.622	15					Integr.	Normal
19	K KA1	Mine15	3.314	15					Integr.	Normal

Default → Special ... Delete group Update cal reference in lib. Update cal reference in FCL

Copy group Clear drift correction data... Undo changes in master Exit

# Line Library Access #2



In application → Measurement section → Line Parameters  
Click on Launch

ApplicationWizard - [DualSoilPaperBags.evm]

File Edit View Method Calibration Window Options Help

DualSoilPaperBags

- Materials
- Preparation
- Prepared Standards
- Measurement
  - Measurement Method
  - Measure Standards
  - Line Parameters
- Calibration
- Modules
- Limits Check
- Results Formatting
- Application
- S2 Ranger Application

Current material : Mining-40kV

Launch

### Line Parameters

**Purpose**  
Modification of the line library (S2-LineLibrary.FLL file).

**Overview**  
A given spectral line (e.g. Al K $\alpha_1$ ) can be measured using different measurement parameters (high voltage of the generator, filter, amplifier settings) and different evaluation parameters (peak/background or spectrum fitting model, sensitivity). A "line" is a set of parameters, has a specific name (that includes the name of the spectral line) and is stored in the line library (there are several lines for a given spectral line, e.g. Al KA1-HS-Min, Al KA1-HR-Min). It is possible to check the lines (display previously measured data), and to adjust the parameters.

**How?**  
The display of measured spectra and the change of the parameters of a line are made by an external program called S2LineEditor. Click on **Launch** and ApplicationWizard will open S2LineEditor for you.

**Note**  
The lines are chosen with **Measurement Method** (previous step), in the Lines tab. Precalibrated lines cannot be modified. Specific lines for a given material can be created with **Measurement Method** (previous step), in the Lines Selection tab. To make the drift correction procedure easier, it is recommended not to create new specific lines unless the existing ones are not adequate. Note that there is a difference between the terms "spectral line" (usual physical meaning) and "line" (entry of the line library, set of parameters, in SPECTRA<sup>EDX</sup>).

S2 Line Editor

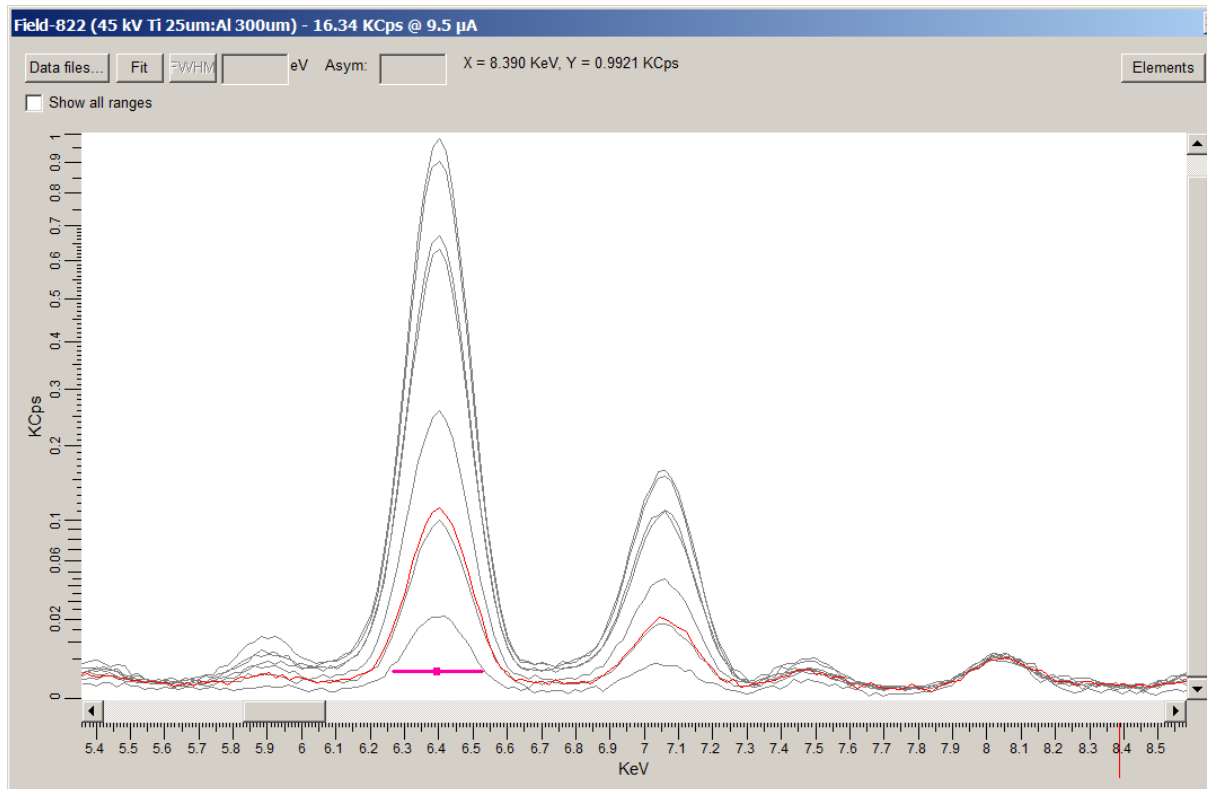
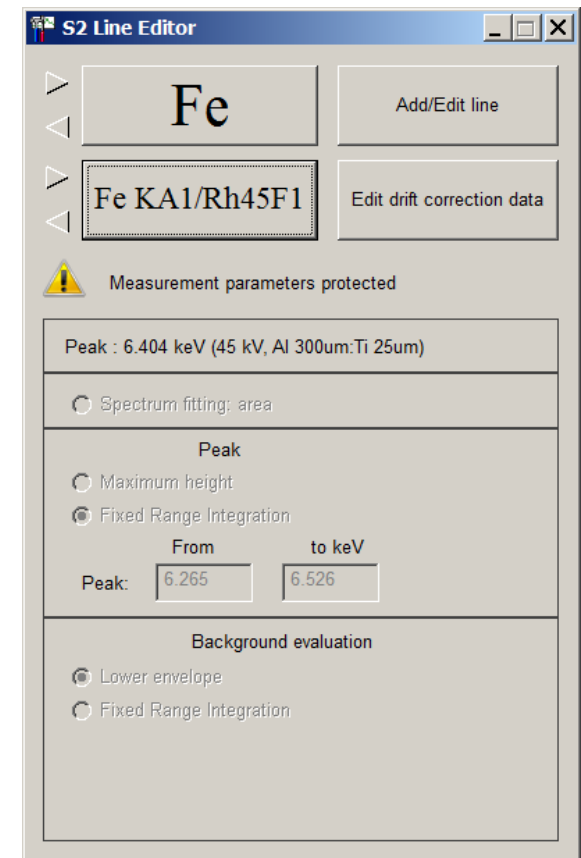
Na

Na KA1/C 114

Peak: 1.017 1.022

# 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



**Path where standards must be (last folder is named for preparation)**

**Problems noted here**

**Multiple preparations**

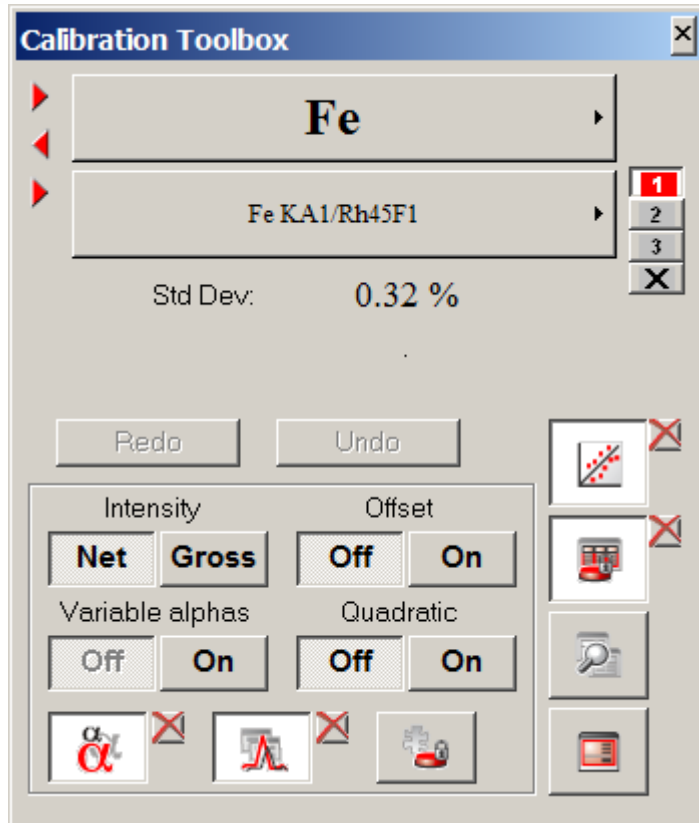
Prepared standards	Imported	Material	Preparation	File
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45HWOE_213	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45W_2a	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45OLO_1	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45DNC_1a	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45DTS_2b	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45GSP_2	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45BHV_2	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45AGV_2	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45GSS_5	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45GXR_1	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45GXR_4	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45SU-1b	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45SiO2_Au50	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45SiO2_Au100	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45SiO2_Au500	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45SiO2_Au1000	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45MP-1b	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45AMIS015	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45AMIS022	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45SRM694	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	M45SY_3	Imported Mining-40kV	Mining-40kV Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Field-054	Imported Mining-40kV	MiningPaperBags Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Field-065	Imported Mining-40kV	MiningPaperBags Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Field-266	Imported Mining-40kV	MiningPaperBags Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Field-394	Imported Mining-40kV	MiningPaperBags Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Field-523	Imported Mining-40kV	MiningPaperBags Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Field-528	Imported Mining-40kV	MiningPaperBags Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Field-816	Imported Mining-40kV	MiningPaperBags Exist
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Field-822	Imported Mining-40kV	MiningPaperBags Exist

# Elements Screen with Toolbox



The screenshot displays the Bruker ApplicationWizard software interface. The main window shows a periodic table of elements with several elements highlighted in grey boxes: 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, Compton, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Rayleigh, Th, Pa, U, Np, Pu, Am. A 'Calibration Toolbox' window is open in the bottom right corner, showing the selected element 'Cu' with a 'Cu KA1/Rh45F1' filter. The standard deviation is 0.0064%. A warning icon indicates 'Stat. error dominates standard deviation.' The toolbox also includes buttons for 'Redo', 'Undo', 'Intensity', 'Offset', 'Net', 'Gross', 'Off', 'On', 'Variable alphas', and 'Quadratic'. The software title bar reads 'ApplicationWizard - [DualSoilPaperBags.evm:1 \*]' and the menu bar includes 'File', 'Edit', 'View', 'Method', 'Calibration', 'Window', 'Options', and 'Help'. The status bar at the bottom indicates 'For Help, press F1'.

# Toolbox Functions

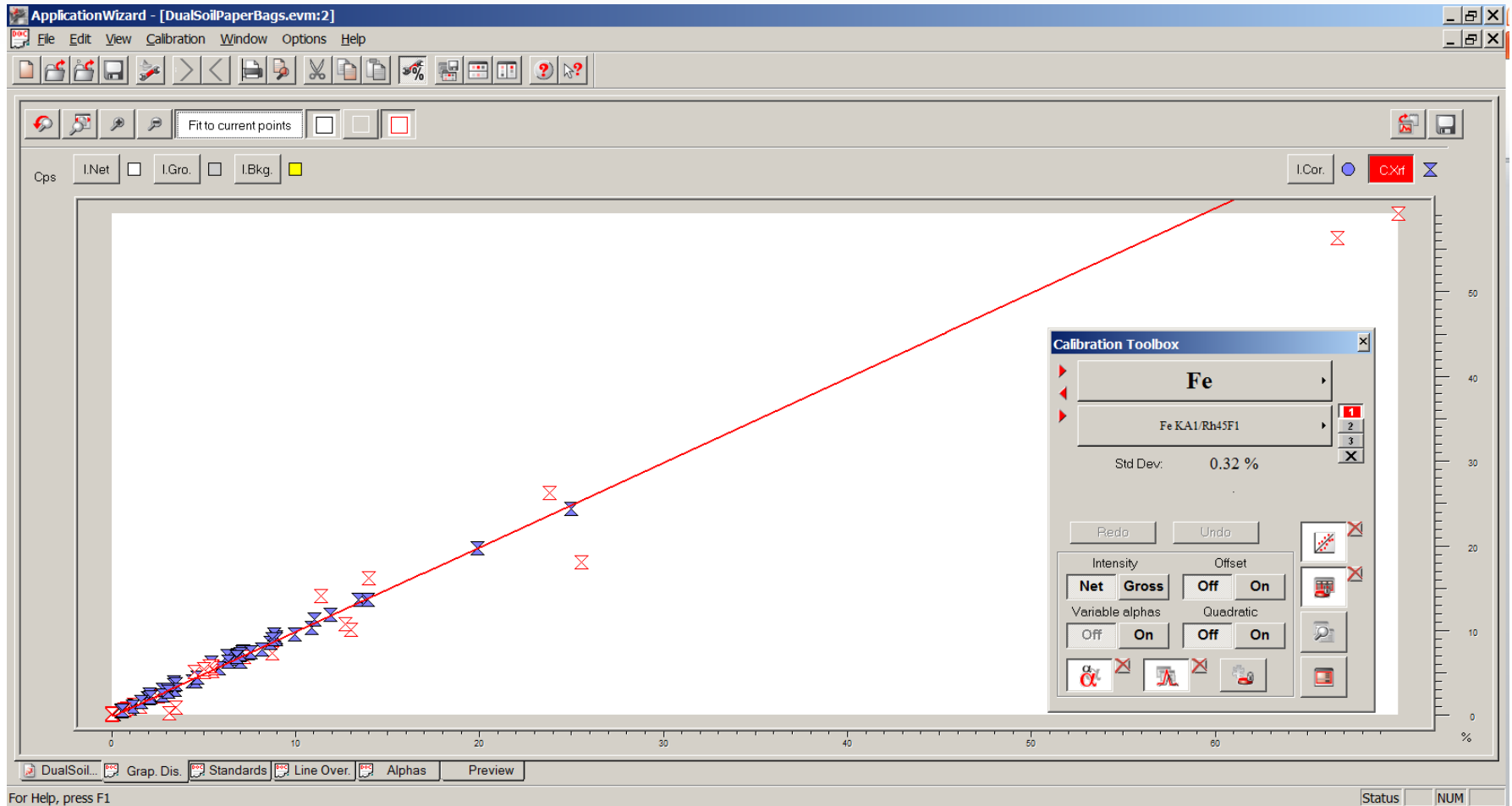


- Switch between screens
- Control offset and quadratic
- Undo/redo
- Control element and line used
- Monitor standard deviation

## Available Screens

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

# Graph Screen with Toolbox



# Standards (Tabular Display) Screen with Toolbox



ApplicationWizard - [DualSoilPaperBags.evm:3]

File Edit View Calibration Window Options Help

Num...	Standard Nam...	Corrected Inte...	Net Inten...	Chemical Concen...	XRF Concentr...	Absolute Devi...	Relative Devi...	LLD (P...
90	M45AGV_2	288.3	254.5	4.680	4.505	-0.175	-3.7	23.5
22	M45AK396	35.5	35.0	0.575	0.554	-0.021	-3.6	33.6
23	M45AK397	44.7	43.8	0.749	0.699	-0.011	-1.6	28.8
24	M45AK401	70.3	68.9	1.124	1.098	-0.026	-2.3	28.7
25	M45AK402	31.6	31.0	0.520	0.493	-0.027	-5.2	27.8
26	M45AK408	51.8	50.9	0.815	0.810	-0.005	-0.67	30.0
27	M45AK411	35.2	34.9	0.539	0.551	0.021	3.9	33.3
28	M45AK423	41.9	41.3	0.699	0.655	-0.035	-5.0	25.7
35	M45AK426	29.9	29.5	0.529	0.467	-0.053	-10	23.3
13	M45AMIS008	574.4	477.0	8.713	8.976	0.263	3.0	30.6
14	M45AMIS013	576.0	479.7	8.951	9.000	0.049	0.55	30.8
15	M45AMIS014	728.3	462.8	11.007	11.380	0.373	3.4	41.5
100	M45AMIS015	359.3	251.0	5.846	5.615	-0.232	-4.0	29.4
101	M45AMIS022	446.5	325.9	6.297	6.977	0.680	11	30.9
54	M45AMIS027	871.3	475.5	13.778	13.614	-0.164	-1.2	49.6
16	M45AMIS031	404.8	410.5	6.357	6.325	-0.032	-0.50	29.9
17	M45AMIS032	440.4	448.0	6.811	6.882	0.070	1.0	32.7
55	M45AMIS034	484.6	404.8	7.161	7.573	0.412	5.7	27.9
56	M45AMIS036	128.8	122.9	1.944	2.013	0.069	3.6	22.7
18	M45AMIS056	465.9	364.8	7.021	7.280	0.259	3.7	28.6
53	M45AMIS060	430.5	349.5	6.636	6.727	0.090	1.4	28.0
19	M45AMIS063	871.8	477.2	13.916	13.622	-0.294	-2.1	46.7
57	M45AMIS064	451.6	378.0	6.699	7.056	0.356	5.3	27.9
20	M45AMIS071	101.8	98.9	1.608	1.590	-0.018	-1.1	20.5
21	M45AMIS072	141.2	134.8	2.098	2.206	0.108	5.1	22.4
58	M45AMIS124	477.9	372.5	7.126	7.467	0.341	4.8	27.9
36	M45BCS176_2	455.6	689.6	6.860	7.119	0.259	3.8	32.4
38	M45BCSAICaFe...	1684.0	1109.8	23.797	26.313	2.516	11	38.1
40	M45BCS_Bauxit...	904.0	877.6	11.399	14.125	2.727	24	25.7

Double-click: enable or disable standard.

Squared correlation coefficient: 0.995773

Regression weighting: Abs Rel Dev Auto

Disable traces Invert selection

Calibration Toolbox

Fe

Fe KA1/Rh45F1

Std Dev: 0.32 %

Redo Undo

Intensity Offset

Net Gross Off On

Variable alphas Quadratic

Off On Off On

→PPM

→Prepared elements

DualSoil... Grap. Dis. Standards Line Over. Alphas Preview

For Help, press F1

Status NUM



# Overlaps Screen with Toolbox

The screenshot shows the 'ApplicationWizard' software interface. The main window displays a table of overlaps with the following data:

Overlap	Energy	Delta...	Remark	Type	Base for calculation ^	Adjust...	Coefficient
Hf LA1	7.899	0.149		Measured	Hf LB1/Rh45F1	Adjust...	-0.3601
Ni KB1	8.267	0.219		Measured	Ni KA1/Rh45F1	Adjust...	-0.04281
Pb LA1	10.550	2.502		Measured	Pb LB1/Rh45F1	Adjust...	-0.02041
Ta LA1	8.146	0.098		Measured	Ta LB1/Rh45F1	Adjust...	-0.5055

The 'Calibration Toolbox' window is open, showing settings for 'Cu'. The current calibration is 'Cu KA1/Rh45F1' with a 'Std Dev.' of 0.0064 %. A warning icon indicates 'Stat. error dominates standard deviation.' The toolbox includes buttons for 'Redo' and 'Undo', and options for 'Intensity' (Net, Gross, Off, On), 'Variable alphas' (Off, On), and 'Quadratic' (Off, On). There are also icons for 'α', 'A', and 'R'.

At the bottom of the main window, there is an information icon and the text: 'To modify an item, click right on it to insert a new item click right in an empty part of the list.'

The status bar at the bottom shows 'DualSoil...', 'Grap. Dis.', 'Standards', 'Line Over.', 'Alphas', 'Preview', 'Status', and 'NUM'.

# 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

The screenshot shows a dialog box titled "Overlap correction for Fe KA1/Rh45F1 (6.404 keV)". The dialog has a blue header bar with a close button (X) on the right. The main area is light gray and contains the following controls:

- Overlapping line:** A text input field with a dropdown arrow on the right.
- Correct by:** A dropdown menu currently set to "Measured", followed by another empty text input field with a dropdown arrow.
- Factor:** A text input field, followed by two radio buttons: "Given" (unselected) and "Adjustable" (selected).
- Search parameters:** A section enclosed in a rounded rectangle containing:
  - Min concentration:** A slider control with a value of "1000PPM" displayed in a text box to the right. A checked checkbox labeled "Escape peaks" is to the right of the text box.
  - Distance (eV):** A slider control with a value of "300" displayed in a text box to the right. A checked checkbox labeled "Sum peaks" is to the right of the text box.

Buttons for "OK" and "Cancel" are located on the right side of the dialog.

# Alphas Screen with Fixed Alphas



ApplicationWizard - [DualSoilPaperBags.evm:5]

File Edit View Calibration Window Options Help

Name	Z	Concentrations		Influence	Variable alphas		Fixed alphas (concentrations)			Fixed alphas (int)
		Min	Max		Min	Max	Theoretical		Empirical	Empirical
H	1	0.0	3.1	0.031	0.000	0.000	-0.995	Fixed	0.000	
C	6	0.0	13.6	0.100	0.000	0.000	-0.730	Fixed	0.000	
O	8	0.0	58.3	0.198	0.000	0.000	-0.341	Fixed	0.000	
Na	11	0.0	6.2	0.036	0.000	0.000	0.586	Fixed	0.000	
Mg	12	0.0	29.8	0.322	0.000	0.000	1.081	Fixed	0.000	
Al	13	0.0	27.9	0.422	0.000	0.000	1.512	Fixed	0.000	
Si	14	0.0	97.7	2.089	0.000	0.000	2.138	Fixed	0.000	
P	15	0.0	13.2	0.348	0.000	0.000	2.643	Fixed	0.000	
S	16	0.0	44.9	1.528	0.000	0.000	3.406	Fixed	0.000	
Cl	17	0.0	2.5	0.099	0.000	0.000	3.942	Fixed	0.000	
K	19	0.0	12.8	0.687	0.000	0.000	5.369	Fixed	0.000	
Ca	20	0.0	31.3	0.000	0.000	0.000	0.000	Fixed	0.000	
Ti	22	0.0	59.8	0.371	0.000	0.000	-0.621	Fixed	0.000	
V	23	0.0	56.2	0.348	0.000	0.000	-0.620	Fixed	0.000	
Cr	24	0.0	68.4	0.403	0.000	0.000	-0.589	Fixed	0.000	
Mn	25	0.0	77.5	0.423	0.000	0.000	-0.546	Theoretical	-0.546	
Fe	26	0.0	69.9	0.316	0.000	0.000	-0.451	Computed	-0.946	
Co	27	0.0	72.4	0.252	0.000	0.000	-0.349	Fixed	0.000	
Ni	28	0.0	78.7	0.140	0.000	0.000	-0.178	Fixed	0.000	
Cu	29	0.0	79.8	0.038	0.000	0.000	-0.048	Fixed	0.000	
Zn	30	0.0	80.3	0.159	0.000	0.000	0.198	Theoretical	0.198	
As	33	0.0	75.8	0.800	0.000	0.000	1.056	Fixed	0.000	
Se	34	0.0	55.2	0.710	0.000	0.000	1.288	Fixed	0.000	

**Calibration Toolbox**

Ca

Ca KAl/Rh45F1

Std Dev: 0.20 %

Redo Undo

Intensity Offset

Net Gross Off On

Variable alphas Quadratic

Off On Off On

H 0.0 3.1 0.031 - - -0.995 >> 0.000

Current 0.0 31.2 No Correct. Computed Fixed Computed Fixed

Ca regression weighting: Abs Rel Dev Auto

Main coefficients: Slope: 0.2512 %/Cps Offset: 0.0 Cps Quadratic: -0.8942

Computed Fixed Computed Fixed Computed Fixed

DualSoil... Grap. Dis. Standards Line Over. Alphas Preview

For Help, press F1 Status NUM





# Alphas Screen with Variable Alphas

ApplicationWizard - [DualSoilPaperBags.evm:5]

File Edit View Calibration Window Options Help

Name	Z	Concentrations		Influence	Variable alphas		Fixed alphas (concentrations)		Fixed alphas (int)	
		Min	Max		Min	Max	Theoretical	Empirical	Empirical	
H	1	0.0	3.1	0.031	-0.987	-0.985	-0.986			
C	6	0.0	13.6	0.135	-0.989	-0.988	-0.988			
O	8	0.0	58.3	0.571	-0.981	-0.980	-0.980			
Na	11	0.0	6.2	0.059	-0.959	-0.957	-0.957			
Mg	12	0.0	29.8	0.281	-0.946	-0.943	-0.944			
Al	13	0.0	27.9	0.259	-0.934	-0.930	-0.931			
Si	14	0.0	97.7	0.890	-0.915	-0.910	-0.911			
P	15	0.0	13.2	0.118	-0.898	-0.893	-0.894			
S	16	0.0	44.9	0.389	-0.873	-0.867	-0.867			
Cl	17	0.0	2.5	0.021	-0.854	-0.846	-0.847			
K	19	0.0	12.8	0.100	-0.793	-0.783	-0.784			
Ca	20	0.0	31.3	0.232	-0.753	-0.741	-0.742			
Ti	22	0.0	59.8	0.410	-0.699	-0.685	-0.686			
V	23	0.0	56.2	0.365	-0.664	-0.648	-0.649			
Cr	24	0.0	68.4	0.406	-0.612	-0.593	-0.594			
Mn	25	0.0	77.5	0.427	-0.570	-0.549	-0.551			
Fe	26	0.0	69.9	0.340	-0.509	-0.485	-0.487			
Co	27	0.0	72.4	0.318	-0.462	-0.436	-0.439			
Ni	28	0.0	78.7	0.278	-0.380	-0.350	-0.353			
Cu	29	0.0	79.8	0.254	-0.348	-0.316	-0.319			
Zn	30	0.0	80.3	0.200	-0.281	-0.246	-0.249			
As	33	0.0	75.8	0.054	-0.111	-0.067	-0.071			
Se	34	0.0	55.2	0.009	-0.059	-0.012	-0.016			

**Calibration Toolbox**

**Rh**

Rh KB1/Mine45

Std Dev: 0.0085 %

Redo Undo

Intensity Offset

Net Gross Off On

Variable alphas Quadratic

Off On Off On

H	0.0	3.1	0.031	-0.987	-0.985	>>		
Current	0.0	0.1				No Correct	Computed	Fixed

Main coefficients:

regression weighting: Abs Rel Dev Auto

Slope: 0.00042 %/Cps Offset: 0.0 Cps Quadratic: 0

Computed Fixed Computed Fixed

DualSoil... Gap. Dis. Standards Line Over. Alphas Preview

For Help, press F1

Status NUM

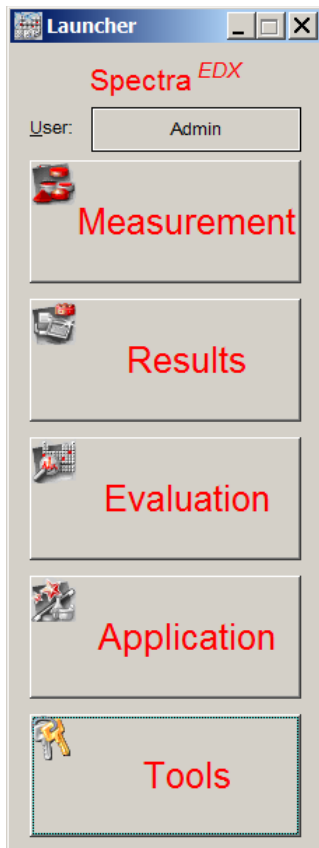
# Completion of the Calibration Curves



- 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

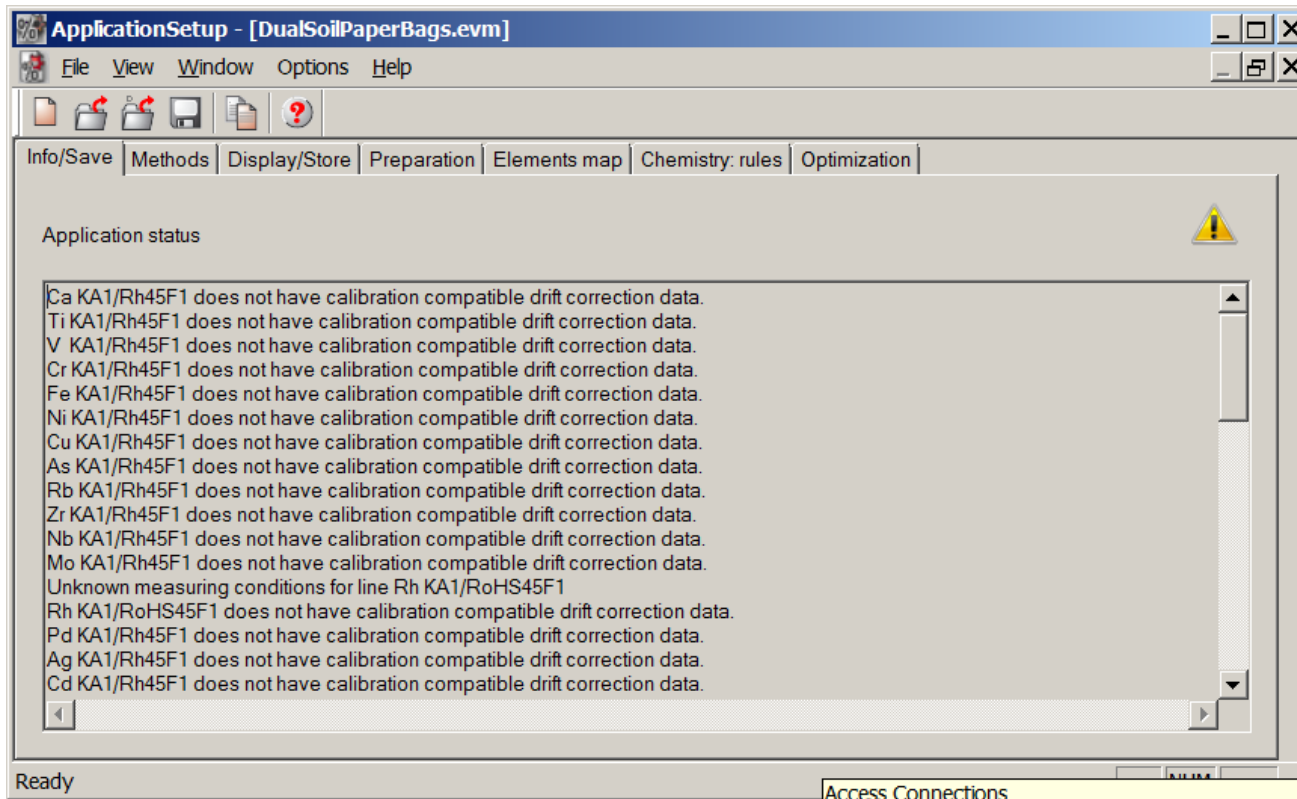
# Opening an evm file



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

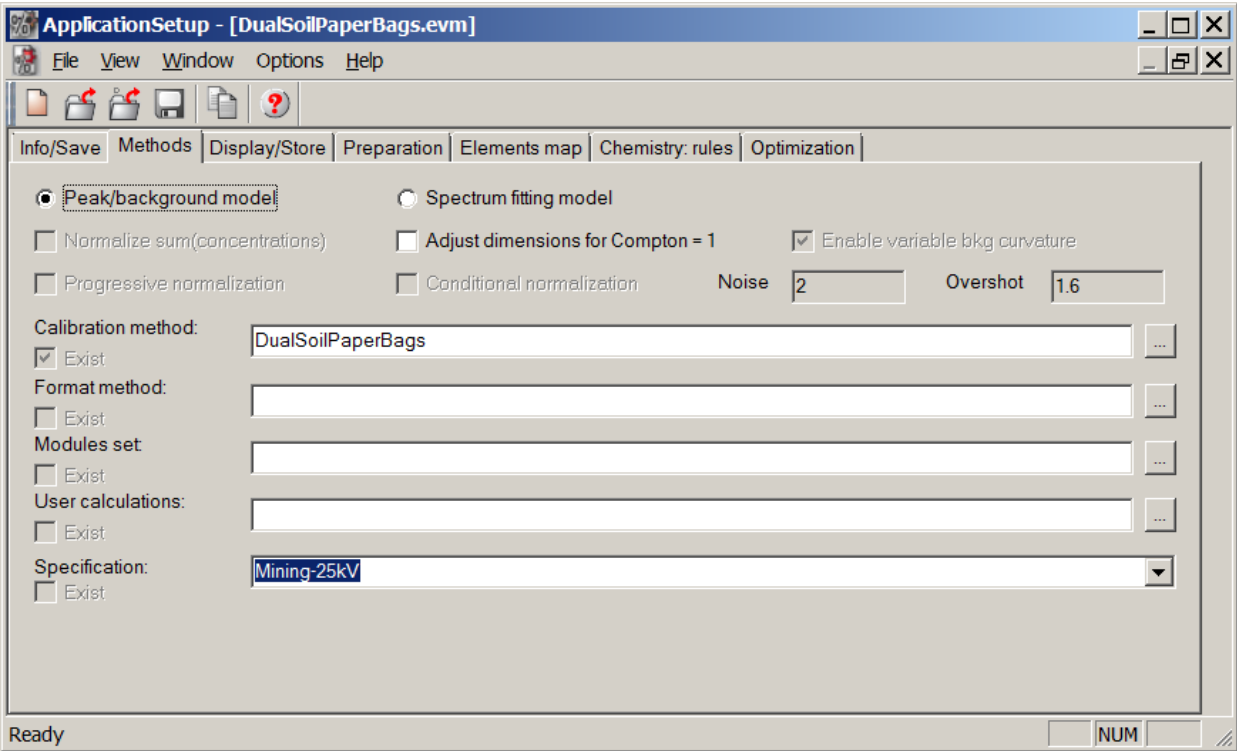
# "Save" Screen With Error Reporting

- 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



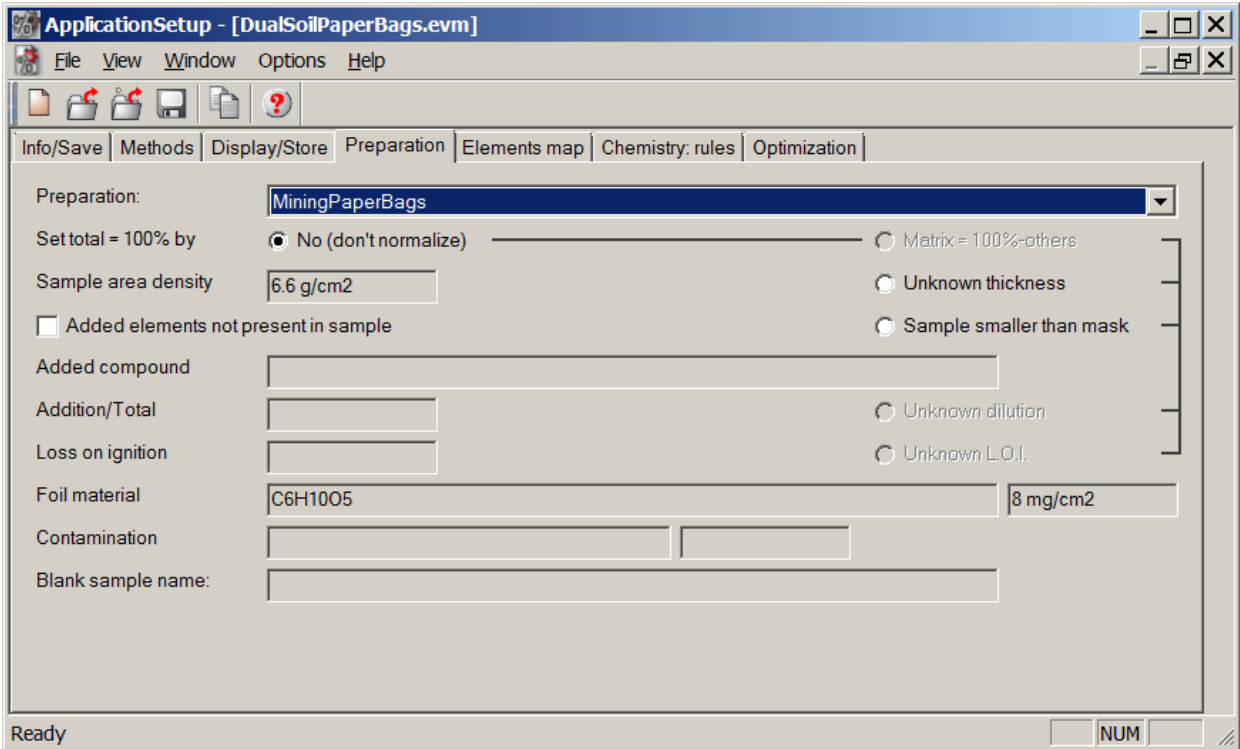
# Methods Screen

- 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

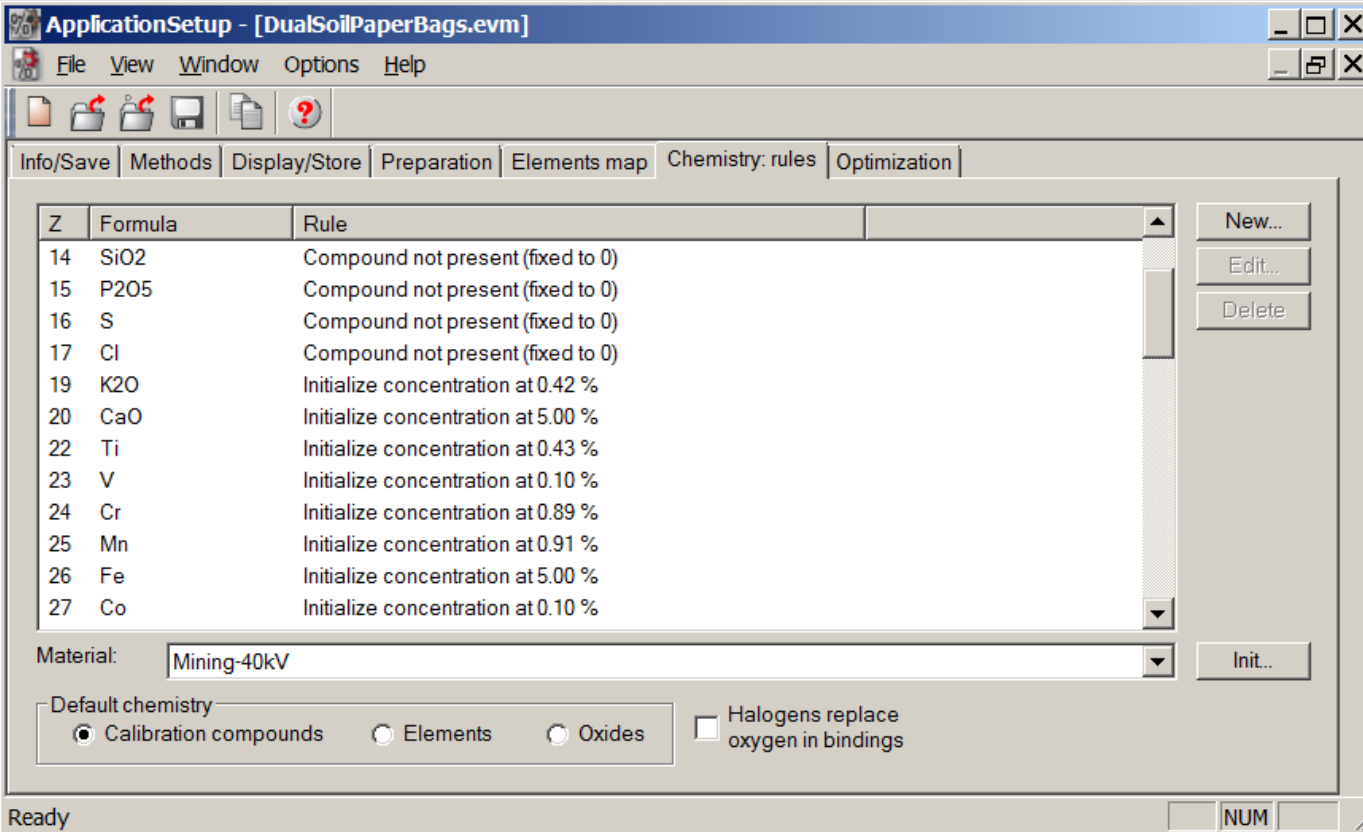
- Choose a preparation from the list (created in Application Wizard)
- Preparation must match the unknowns to be measured
- Normalization is not used much in geo applications because of “invisible” elements like C, O, N, etc.





# “Chemistry: rules” Screen

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

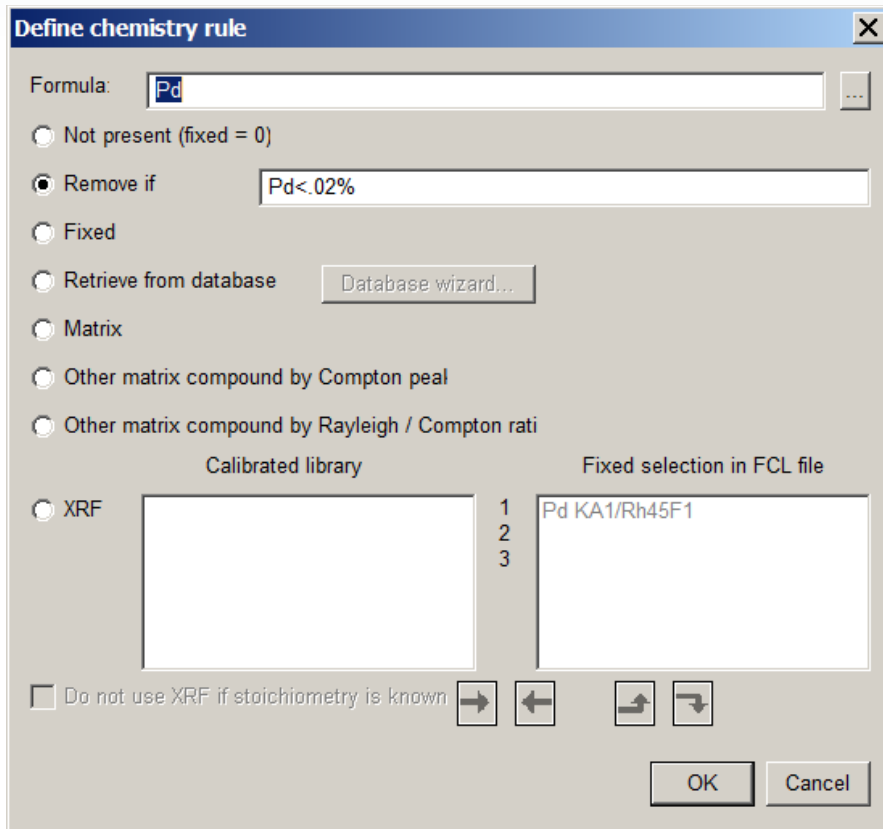


Z	Formula	Rule
14	SiO2	Compound not present (fixed to 0)
15	P2O5	Compound not present (fixed to 0)
16	S	Compound not present (fixed to 0)
17	Cl	Compound not present (fixed to 0)
19	K2O	Initialize concentration at 0.42 %
20	CaO	Initialize concentration at 5.00 %
22	Ti	Initialize concentration at 0.43 %
23	V	Initialize concentration at 0.10 %
24	Cr	Initialize concentration at 0.89 %
25	Mn	Initialize concentration at 0.91 %
26	Fe	Initialize concentration at 5.00 %
27	Co	Initialize concentration at 0.10 %

Material: Mining-40kV

Default chemistry:  Calibration compounds  Elements  Oxides  Halogens replace oxygen in bindings

# 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

ApplicationSetup - [PrecMetals.evm]

File View Window Options Help

Info/Save Methods Display/Store Preparation Elements map Chemistry: rules Optimization

Filtering options for questionable data

- Filter peaks Intensity threshold: 3\*sigma
- Use negative intensities
- Discard excessive intensities

	TR lines	Default lines	Maj lines	Maximum
Proportional counter KCps	100	200	500	6000
Scintillation counter KCps	100	150	300	6000

- Discard line when overlap > % of measured intensity
- Ignore missing overlap error
- Trim negative concentrations before absorption calculations

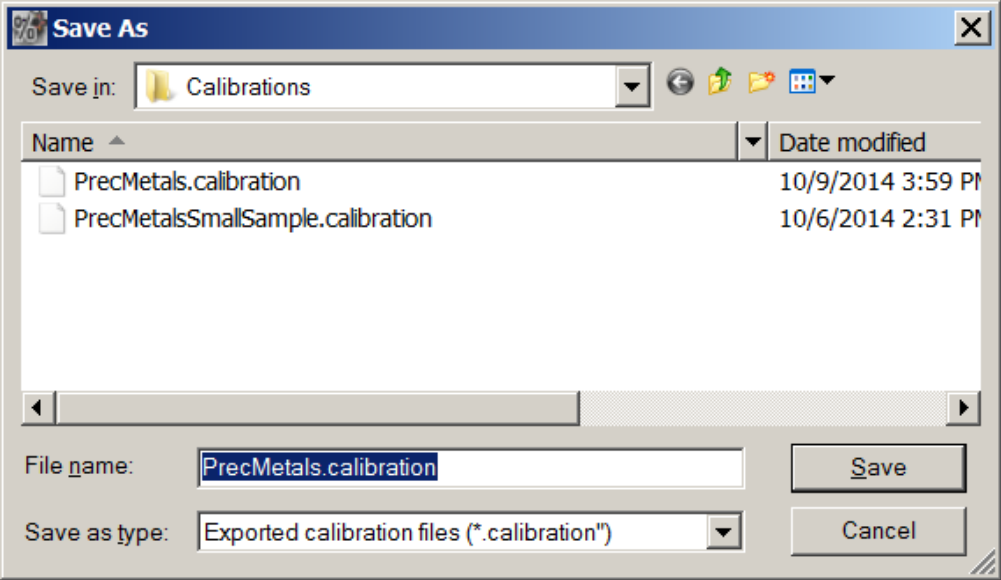
Iteration control

- Maximum number of cycles (normal evaluation): 5
- Maximum number of cycles (optimized or multilayer): 5
- Error threshold to exit iteration loop (in % of calc. value): 0.1 %

Ready NUM

# Saving as a .calibration File

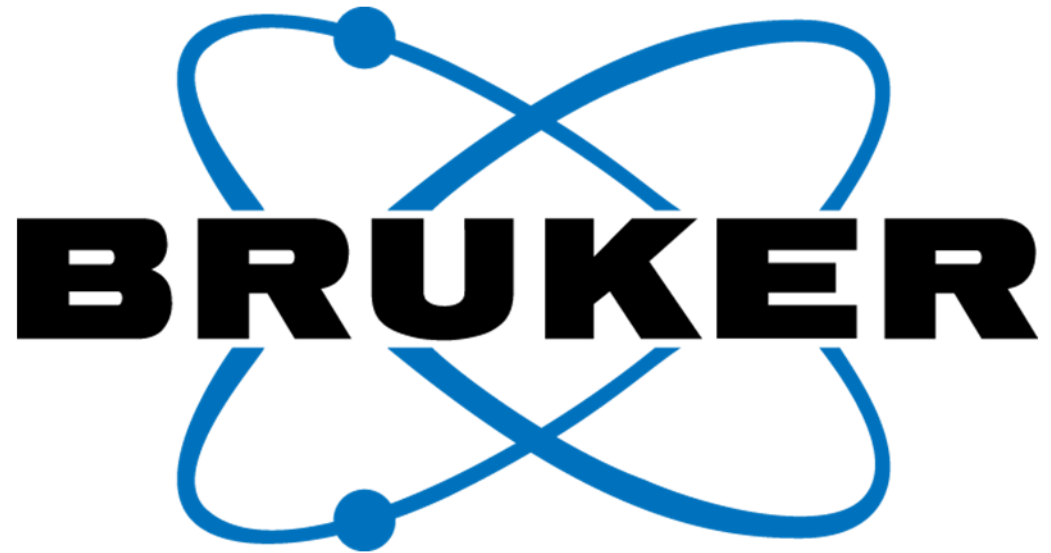
- Click on “File” and choose “Export to calibration file” from the drop-down menu
- The screen below will appear
- Choose an existing file to save over or create a new one by typing in the name at the bottom
- The .calibration file is what is transferred to the instrument





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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