

Creating Empirical Calibrations

Spreadsheet Manual

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1. Overview

1.1. It is important to understand the logical process of the S1 Bruker program on the Tracer's PDA. In order for the program to select the correct chemistry coefficient file, it must first identify the <u>analyte matrix</u>, then the <u>alloy grade (or general composition)</u>. To do this, the program initially looks for the major K-shell peak intensity (the matrix element), and then places the analyte in a matrix category ("Class", e.g., Fe, Co, Ni). Next, the program analyzes the intensity ratios of the characteristic elements for the alloy matrix-set to determine Grade ID. For alloys, this is the 12-16 elements that the industry uses to identify a particular Grade ID (e.g., stainless steel 304 or 321). The program can then point to the correct chemistry coefficient file (".cfz") and calculate the chemistry composition of the sample.



- 1.2. When creating calibrations for other materials, you must decide the elements that are critical to differentiating one specimen from another. For field analysis, this will allow you to shoot a variety of samples without having to manually pre-select the calibration you wish to use. This is the "Sort" or "Grade ID" calibration ("*.srz").
- 1.3. Finally, when the program has detected sufficient data to classify the analyte, it will use the associated calibration coefficients stored in the, *"*.cfz"* file, to output quantitative chemistries for the elements of interest.
- 1.4.

Note

The default chemistry calibration uses Region of Interest (ROI). To use a Compton ratio, you must select Compton in the Chem model of the spreadsheet <u>AND</u> change columns "E" and "F" in the Alloy.csv file.



2. Enable S1 Calibration Macro

Note

- Enabling the S1 Calibration Macro adds a tab to the Excel menu bar.
- The calibration spreadsheet provided on the CD has all of the original alloy calibration spectra files already loaded (over 250 assays). Spectra files have the extension, "**.pdz**".
- The "Read PDZ" function is used strictly to perform the initial factory calibration and reads all 250+ pdz files into the spreadsheet.

2.1. For Use with Excel 2003 or Earlier

- 2.1.1. **OPEN** the calibration spreadsheet.
- 2.1.2. In the Excel menu bar, **CLICK** *Tools*.
- 2.1.3. **SELECT** Add-ins.
 - 2.1.3.1. If the KTI Calibration Macro appears in the Add-in list, **ENSURE** box is checked.
 - 2.1.3.2. If box is not checked, **CLICK** *Browse* <u>AND</u> <u>THEN</u> **SELECT** the file *C:\Program Files\KTICommon\S1CalMacros.xla* <u>AND</u> <u>THEN</u> **CLICK** OK.
- 2.2. **CLICK** OK on the Add-Ins box. The S1CalProcess item should appear in the Excel menu bar.

2.3. For Use with Excel 2007

- 2.3.1. **OPEN** the calibration spreadsheet.
- 2.3.2. CLICK the Microsoft Icon in upper left corner 🖲.
- 2.3.3. **SELECT** Excel Options.
- 2.3.4. **SELECT** *Add-ins*.
 - 2.3.4.1. If the KTI Calibration Macro appears in the Add-in list, **CLICK** OK.
 - 2.3.4.2. If box is not checked, **CLICK** *Browse* <u>AND</u> <u>THEN</u> **SELECT** the file *C:\Program Files\KTICommon\S1CalMacros.xla* <u>AND</u> **ADD** Macro to list.

3. Getting Ready

Note

In order to add a new alloy to the calibration, you must have a sample of the new alloy and the laboratory analysis for chemistry of that sample (it is possible to add an alloy to the sort calibration without having the chemistry).

3.1. **ENSURE** the chemistry of the alloy fits within the currently existing calibration range of the instrument you are working on.



- 3.1.1.1. If the assay results are acceptable, **ADD** the sample to the "Sort/Grade ID" calibration. (**Note:** If both the name and assay are correct, there is no need to add this alloy to the calibration).
- 3.1.1.2. If the assay is <u>NOT</u> acceptable, **ADD** this sample to both the Sort and Chemistry calibration.
- 3.2. **REVIEW** the chemistry of the alloy to be added <u>AND</u> **DETERMINE** the proper chemistry model to which it should be added. The existing assay models for the standard Alloy instrument include:
 - TS1 Tool Steels
 - NI1 Ni which are not included in Ni2 or Ni3
 - NI2 Ni alloys with high Co
 - NI3 Ni alloys with high Mo
 - FE1 Low alloy Irons
 - FE2 Stainless Steels (i.e., Fe based alloys with more than 5% Cr)
- CO1 All cobalt alloys
- CU1 All Copper Alloys
- TI1
- TI2
- TI3
- TI4

4. Measuring the New Sample

WARNING

- RADIATION HAZARD. X-RAYS EMITTED.
- BECAUSE THE SOFTWARE CONTROLS THE TRIGGER, IF THERE IS A SAMPLE ON THE INSTRUMENT AND THE IR SAFETY SENSOR IS COVERED, PXRF WILL START THE ASSAY.

Note

If the sample is an alloy, take a test assay in portable mode using the S1 Bruker program on the PDA. Note the matrix and alloy ID given. This will help to categorize and select the correct calibration method group. The actual calibration assays can also be taken in portable mode, but since the assays are long, it is usually easier to take them with the instrument in "Lab Mode", (connected to the PC and using PXRF). For instructions on taking timed assays, see the Tracer Series User Guide

- 4.1. **PLACE** the S1 Tracer in its stand with AC power or battery.
- 4.2. **TURN** the Tracer power switch on.
- 4.3. **CONNECT** the serial cable to the Tracer and PC.
- 4.4. **OPEN** the PXRF program on the PC.



- 4.5. **PLACE** the sample on the TRACER aperture
 - 4.5.1. If the sample is small or low density, **COVER** sample with safety shield.
- 4.6. **SELECT** the desired instrument parameters from the "KTI Tube" menu. (Note: alternately, you may **SELECT** PC Trigger box, if available).
- SELECT "Timed Assay" from the PXRF "Timed" menu.
- 4.8. ENTER the desired assay time. (The sample should be measured for at least 120 seconds (180 seconds is better), and for aluminums, 180 seconds is minimum.
- 4.9. Select "OK".
- 4.10. **ENTER** a file name designating the sample ID.

5. Adding New Standards to the PDZFiles Sheet

- 5.1. **OPEN** the "PDZ Files" tab (Figure 1).
- 5.2. **ENSURE** elements of interest are present on the list of elements.
 - 5.2.1. If not, **SELECT** the last element column, **COPY** <u>AND</u> **INSERT** it as a new column at the end of the element columns.
 - 5.2.2. **RENAME** the column to the desired element and atomic shell (e.g., BiLb1).
- 5.3. From the Excel menu bar, **SELECT** <u>*Ca*</u>*Process* (Figure 2).
 - 5.3.1. **SELECT** *Insert PDZ Files*. This will bring up the window with the serial number of the instrument (Figure 3).
- 5.4. **ENSURE** serial number is the correct one for the instrument
- 5.5. **UNCHECK** *Remove sort corrections* (Figure 3).
- 5.6. **CLICK** OK. A file selection window opens (Figure 4).

220	13	55 JU8L		reizo
221	1	Nitronic 30		Fe129
222	:	Ss 465		Ss465
223	:	Ss 420		Ss420
224	:	5s316		Ss316
225	:	5s22135		Ss22135
226	:	5521103		ss21103
227	1	Biodr108		Biodr108
228				Range1
229	1	ron-27A		fe001
230		Aisi 1018		fe002
231		Aisi 1030		fe 12
4	H	AlloyDesc /	PDZFiles	A 15Sort

Figure 1









Figure 4



5.7. **SELECT** all *.pdz files to be added and **CLICK** Open. The spreadsheet will automatically load all of the selected data.

6. Sort I: Adding or Removing an Alloy to an Existing Sort Calibration

Note
Even if your main interest is to add to the
chemistry model, the new sample should be
added to the Sort model.

- 6.1. In Excel, **SELECT** the Sort sheet appropriate for the matrix.
- 6.2. From the S1 CalProcess menu, **SELECT** *Add/Remove Elements* <u>AND</u> **CHANGE** the elements of interest as desired.
- 6.3. From the S1CalProcess menu, **SELECT** Add/Remove Sort Files. A window will open (Figure 5).



Figure 5

Notes

- At least one file must be available at all times so, first <u>add</u> files <u>before</u> removing files.
- Available files (from PDZ sheet) that are NOT currently in use are listed on the left (see Figure 5); files currently in use are listed on the right.
- Multiple files may be selected by holding down the Ctrl key.
- 6.4. **CLICK** on each file you want to ADD.
- 6.5. **CLICK** *Add*. A window will open *with* a Sigma value option.
- 6.6. **DO NOT CHANGE** the Sigma value (default is "2").
- 6.7. Click OK.
- 6.8. **SELECT** any files you wish to eliminate from the "Sort" model.
- 6.9. CLICK Remove.
- 6.10. CLOSE the Add/Remove window.
- 6.11. From the S1 Calibration menu, **SELECT** Create Sort File.
- 6.12. **SAVE** the file to the appropriate folder (this creates the *.srz file [e.g. Fe1.srz]. Each matrix has its own sort model).
 - 6.12.1. If you receive a "Sort Range Error" showing overlapping alloys and you **DO** have all of the original calibration PDZ files, **CLICK** *Ignore*.



7. Chemistry I: Adding a New Sample to an Existing Chemistry Model

Notes

- If using a new sample, you will need the laboratory analysis for the sample.
- If using a certified reference material, you will need the certificate.
- Ensure that <u>all</u> of the tube settings in the new spectra are exactly the same as the original spectra used in the present model. (See PDZ Files sheet, columns "BA" to "BL").
- 7.1. Before adding a new alloy or sample to a Chemistry model, **ENSURE** all of the elements of interest are already in the model.
 - 7.1.1. If all samples are NOT present, GO TO the PDZ file sheet and ENSURE the elements and lines are there.
 - 7.1.1.1. If the element and/or line IS NOT in the list, ADD it to PDZfiles sheet as described in Appendix A).



Figure 6

- 7.2. From the S1CalProcess menu, **SELECT** *Add/Remove Elements* .
- 7.3. **ADD** the new Element or line.
- 7.4. SELECT Add/Remove Chemistry Files. A window will appear (Figure 6).
- 7.5. **SELECT** the new sample from the *PDZ List* on the left.
- 7.6. Click *Add*.

Note

After adding the new "pdz" files (spectra) to the Chemistry model, you will automatically be shifted to the portion of the spreadsheet to enter the chemistry values (Lab results) for the new standard; if this does not happen, the area is located at the far right of the Chemistry sheet.

7.7. **ENTER** the laboratory assay value or certified value for each element as a wt% (without the "%") for alloys or appropriate unit of measure. (**NOTE**: These should be elemental concentrations, not oxides).

Note Assay values may be added as each sample is added, or added later when other tasks are completed.

- 7.8. **ENTER** the assay values for the sample.
- 7.9. From the S1CalProcess menu, **SELECT** Create Chemistry files.
- 7.10. **SELECT** the appropriate chemistry calibration model (e.g., Cu1) (Figure 7, 1).

Note



When using Compton for Chemistry Intensity, use either the actual Compton energy range (Figure 7, 2), or select any energy range that provides optimal count rate and does not (and will not) have any element intensities.

Create Chemistry files

- 7.11. **SELECT** the Chemistry Intensity (normalization method) (Figure 7, 3):
 - ROI (Regions of Interest) is the default and recommended mode for alloys
 - Compton is typically used for light element matrices and/or thin samples
 - Time (Net Intensities: Time is not recommended as a normalization method)
- 7.12. **CLICK** OK. The Delta-I Model Selection window opens.

🗐 e Chemistry Name Cancel ▲ CU1 * Documents and Settings (1)shannon 🔄 Desktop & Deconvol ion exists Officedocs 🔁 teachingadds 🔁 Calibrations IIIV ΟK * Chem calculated 🔁 Teaching 4 Non-Va Compton Energy Start (kV) 1.13 0KW_860.PDZ 0KW_900.PDZ End (kV) 1.87 0KY_285.PDZ 4KY_270.PDZ UA1.PDZ 14Kʻ 765.PDZ Cher stry Intensity 05001.PDZ ROI 3)-05002.PDZ Figure 7 (1) Chemistry Model (2) Compton Range (3) Intensity Method

7.13. Understanding Delta Model Selection

- 7.13.1. The four columns (parameter options) on the left side of the Delta-Model Selection window (Figure 8) are used to create the regression equation (each element has its own separate coefficients):
 - **Element** is the element currently being calculated/calibrated.
 - **Slope** is selected for elements that may have an absorption/enhancement factor for the element of interest. This correction will be used in the regression to correct the concentration of the selected element. (To select or de-select an element, hold down the "Ctrl" key and click on the desired elements). **Note:** If you do not hold the "Ctrl" key, you will lose the previous selections.
 - **BG S** (Background subtraction) provides a background/overlap correction for the element.
 - **Omit Std** is used if a particular standard appears to be clearly a bad standard (or not appropriate for the calibration), select "Omit Std". **Note**: Be careful about omitting a standard. The problem is usually an interfering element. Omitting a standard in one calibration does not omit it from other elements' calibrations.



Element	Slope	BG S	Omit Std	MnKa1	Given	Calc	Dif
TiKa1	TiKa1	TiKa1*	ni231	ni231	0.11	0.200051	-0.09005
V Kal	V Ka1	V Ka1*	ni232	ni232	1.01	0.963056	0.04694
MoKal	MoKa1	MoKa1	ni233	ni233	1.03	0.962519	0.06748
FeKa1	FeKa1	FeKa1	ni235	ni234	0.77	0.738845	0.03115
CoKa1	CoKa1	CoKa1	ni237	ni235	0.25	0.244786	0.00521
NiKa1	NiKa1	NiKa1	ni238	ni237	0.19	0.027140	0.16286
CuKa1	CuKa1	CuKa1	ni239	ni238	0.067	0.049324	0.01767
Hflh1	Hftht	Hfth1	ni240 ni241 ni243 ni251	ni239	0.2	0.227565	-0.02756
TaLb1	TaLb1	TaLb1		ni240	0.65	0.832319	-0.18231
W Lb1	W Lb1	W Lb1		ni251	ni241	0.45	0.459072
NbKa1	NbKa1	NbKa1	ni262	ni243	0.52	0.528726	-0.00872
MOKal	I MOKAI	Mokal	ni263	ni251	0.68	0.608956	0.07104
			Juner	ni262	0.11	0.117507	-0.00750
🔽 Const.			Cours	ni263	0.025	0.119567	-0.09456
			Save	ni277	0.82	0.802567	0.01743



- 7.13.2. **MONITOR** the progress of the regression calibration by watching the *Ave Dev* at the bottom of the window. In general, a lower value is better.
- 7.13.3. **MONITOR** the error for each standard by observing the table at the right of the window.
- 7.13.4. **DO NOT SELECT** too many elemental corrections or terms for the regression, as this will cause the actual measurement to become unstable and impacts the precision of the measurements from one reading to the next. This is why the *Ave Dev* value is most important when creating a calibration model. (*If the Ave Dev is "Ø", then you have selected too many corrections.*)
- 7.13.5. Once the regression for an element has been completed, **SELECT** the next element in the list. After each element has been calibrated, an asterisk (*) will appear next to the element in the BG S column.
 - 7.13.5.1. To change the correction for some elements, and to save the factory defaults, **USE** the arrow keys ($\downarrow \uparrow$) **TO SCROLL** through the elements after selecting one from the element list. All elements in the list should be addressed before saving the calibration.
 - 7.13.5.2. Once all the elements have been satisfactorily regressed, **CLICK** *Save*. This will bring up a directory selection box.
 - 7.13.5.3. **SELECT** the directory "*C*:\.....*Current Cal*".
 - 7.13.5.4. CLICK Save.

8. PDZFile II: Adding New XRF Lines to PDZFile Sheet

Note



- You will most likely have new samples to use for calibration for this new matrix. It is best to add the new samples into the PDZFiles sheet before editing the *XXSort/XXChem* sheets.
- If you wish to add Element lines that are not already shown in the PDZFile Sheet, it is best to add them first.
- In the following examples, XX is a placeholder for the element of interest and/or its line (e.g., XXXX might be a placeholder for PbLb1). Some date is a placeholder for the date used in a filename.
- 8.1. To add an Element line, **INSERT** a column.
- 8.2. **TYPE** in the new line using the same naming convention (e.g., CrK, AsKb1, PbLb1).
- 8.3. From the S1CalProcess Menu, **SELECT** "Read PDZ File" This will bring up the window with the serial number of the instrument as shown.
- 8.4. **ENSURE** the serial number is correct for the instrument.
- 8.5. **UNCHECK** Remove sort corrections.
- 8.6. **CLICK** OK. A file selection window will then open.
- 8.7. **SELECT** the directory where the currently used data is located (e.g., the Non-vac Alloy data might be found on a CD in the directory "E:\K0XXXX *Some date* Tracer111LE\K0XXXX Non-Vac *Some date*\K0XXXX Non-Vac Data\").
- 8.8. **SELECT** *Read PDZ Files* to reorder all the element lines from lowest to highest energy and calculate the intensities for the added lines.

Note
At least one file must be available at all times so, first <u>add</u> files <u>before</u> removing files.
8.8.1. SELECT Insert PDZ files to add at least two of your new samples

- 8.8.2. **ADD** the samples into the XXSort and XXChem as described in Sections 6 and 7.
- 8.8.3. If the original data is not available, **DELETE** all the file names in the PDZfiles sheet (delete both Column B and A for good housekeeping).

9. Sort II: Adding a new Matrix

	Notes
•	In order for the macros to work properly, the Sort sheet must be created <u>BEFORE</u> creating the Chem
	sheet.
•	There can be multiple calibrations in one chemistry sheet each labeled with the same two letters, defining the major element, and a sequential number to designate the different chemistry calibrations. It would be best to pick a sheet that has the number of chemistry calibrations you plan to make so that you do not need to add or remove calibrations.
•	Adding multiple calibrations is described at the end of the Appendix.

- 9.1. To create a new sheet for the Class (i.e. CuSort/CuChem), **RIGHT CLICK** on an existing XXSort sheet <u>AND</u> **SELECT** *Move or Copy*.
- 9.2. **CHECK** the *Create Copy* box



- 9.3. Click OK.
- 9.4. **REPEAT** Steps 0 through 9.3 for the corresponding XXChem sheet.
- 9.5. **RIGHT CLICK** on existing tabs and **SELECTING** *Rename*.
 - 9.5.1. **RENAME** each sheet with a two letter element name followed by Sort or Chem (e.g., CuSort/CuChem or "K Sort"/K Chem).
- 9.6. In the XXChem sheet, **GO TO** cell A2.
 - 9.6.1. **SCROLL** to the right past the cell with "blank" typed in it and past the second set of XRF lines until you reach a cell with a two letter element designation followed by a number, the two letter designation should be both capital letters for example "AL1".
 - 9.6.2. **CHANGE** the 2 letter designator to match the sheet, but the sheet has one capital and one lower case.
 - 9.6.3. **CHECK** that you are changing a cell that has the text and not a link to a cell with the text.
- 9.7. **REOPEN** the XXSort sheet.
- 9.8. **ADD/REMOVE** sort files in accordance with Section 6.
- 9.9. **RENAME** the Base element column.
- 9.10. **ADJUST** the formulas to recognize the new Matrix or "Base" element.
 - 9.10.1. In area labeled *Adjusted Windows* (below the first area), **RESET** the equations (e.g., if Cu is the new Base and is in column G, then the formulas in the *Adjusted Windows* section should be X/\$G?).
 - 9.10.2. **ENSURE** that the cell above the XRF line (i.e.CuKa1) (located to the right of the *Master Section* and below the *Adjusted Windows* section reads *Base* <u>AND</u> the cells over the XRF line read "If(xx=1000,"Base",""), where xx is the first cell in the matrix column just below the XRF line name.

10. Creating a Flashcard Image

Several files must be updated in order to use the new calibrations on the PDA. The *Build PDA Image* macro will update these files automatically.

11. Transfer Modified Files to Flash Card.

The *Build PDA Image* macro will create a new Flashcard image that contains both the Factory calibrations and the new calibrations.



Appendix A Creating a new Matrix Calibration

- 1. **SELECT** any existing "Sort" spreadsheet.
- 2. **SELECT** "Copy to New Sort Sheet" from the CalProcess Menu.
- 3. **SELECT** any existing "Chemistry" spreadsheet.
- 4. **SELECT** "Copy to New Chemistry Sheet" from the CalProcess Menu.
- 5. **RETURN** to the new "Sort" sheet.
- 6. **ADD** or **REMOVE** Elements from Chemistry spreadsheet.
- 7. **ADD** or **REMOVE** Elements from the sort files.
- ADJUST the formulas to recognize the new Matrix or "Base" element (e.g., if Sn is the new Base and is in column J, then the formulas in the *Adjusted Windows* section should be X/\$J. (IMPORTANT: CHANGE the old Base element column <u>first</u>.)

NOTE: <u>YOU MUST</u> "Create Sort" before using the Chem sheet. None of the Chemistry macros will work until you do so.

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	F48 👻	<i>f</i> ∞ =F3/\$I	F3													
	A B		D	E	F	G	Н	1	J	К	L	М	N	0	P	(
25	25 Ta_456A	T_156A	1537.5371	49000.1021	22162.064	1666.74144	14792.3133	75943.5085	34052.9209	1184.17737						
26	26 Ta_417B	a_417B	1530.9235	344207.835	689.067614	330.658799	245.75885	2724.59064	1492.24743	699.050956						
27	27 Ta_417A	Ta_417A	3506.28647	168944.229	20042.2081	1831.08684	13591.4764	221208.315	3620.82287	616.034891						
28	28 Ta_4	Ta_4	1933.78891	30419.6094	72367.7153	6038.80011	47929.7942	308403.417	3163.82139	774.415871						
29	29 Ta_3	1a_3	2957.96081	34488.9672	53395.3959	5096.2369	36401.7081	364341.366	2876.5158	849.670088						
30	30 Ta_Z	T- 70	449.423438 EEC4.000000	26482.3726	47050.0044	6180.02357	73953.4324	900007.000	1323.774	728.125947						
22	22 To 1	Ta_75	499 101000	92327.1733	97 336, 3399	44/0.22013 COAC CCAA2	40001 0471	200037.000	10202.1700 0000 CECOE	000.07032						
33	33 Ta 8	Ta 8	2890 29501	35906.496	395511738	4396 41573	27364 4711	476598 506	6545 17712	945 543902						
34	34 Ta 74	Ta 74	2116 37937	55401 6994	40465 0061	3755 03445	27170 0914	239125.839	31743 2634	998 578222						
35	35 Ta 417C	Ta 417C	1756 71307	386319.099	1029.98837	453 070791	473.358659	5794 83906	1517.95227	800.903741						
36	36 Ta 457L	Ta 457L	20568.8256	100676.687	4374.38335	1572.23519	4182,91433	119832.339	2181.91735	878.287376						
37	37 Ta_44	Ta_44	3426.58148	41447.6585	48946.0312	4941.40372	34123.7313	326179.489	12345.1032	827.053723						
38	38 Ta_458A	Ta_458A	2578.1073	14880.7501	7390.4124	1180.65853	5282.88597	63634.8222	114419.761	2223.46451						
39	39 Ta_ 1 6	Ta_16	1407.33249	24436.2575	39359.38	4505.95706	27769.3628	487171.102	5319.9784	837.562044						
40	40 T 13	Ta_13	3353.75929	27017.2556	26081.6423	3268.08162	19066.9358	387989.933	23548.9735	885.541593						
41	41 7a_30	Ta_30	3433.19231	39594.2988	63783.6158	6096.53301	43457.7484	339542.975	3745.14266	877.780209						
42	47 Ta_19	Ta_19	3524.43415	40853.6358	33103.5126	6351.52116	29811.5792	463001.118	2886.51986	837.887908						
43	¹³ Ta_15	Ta_15	2246.37942	26394.4184	45145.4959	4663.48223	31094.4362	369837.35	19076.4848	986.434471						
44	44 Ta_40	Ta_40	2276.82378	28513.9547	50080.7626	5301.4931	35203.0954	354412.461	9394.68144	748.978964						
45	Adjusted	d windows														
1			TiKa1	FeKa1	TaLa1	BeLa1	W Lb1	NbKa1	SnKa1	SbKa1						
48	Ta_71	Ta_71	0.02836979	0.62389857	1	0.14790003	0.81800413	6.53024483	0.10637171	0.01392048						
49	Ta_70	Ta_70	0.10527305	100039593	1	0.19446442	0.82480222	5.04030815	0.33015096	0.01859835						
50	Ta_474C	Ta_474C	0.05660088	0.92393268	1	0.18542211	0.90706341	6.84345273	2.61976645	0.07541639						
51	Ta_474B	Ta_474B	0.07255174	3.34816999	1	0.25802927	1.04277123	7.11505378	7.4270848	0.17393898						
52	Ta_474A	Ta_474A	0.04781306	0.46531408	1	0.13914294	0.82763766	5.0136552	1.08532729	0.03622698						
53	Ta_458C	Ta_458C	0.36697179	28.1293979	1	0.27576341	0.68932958	6.02773716	4.3263653	0.65109986						
54	Ta_457Q	Ta_457Q	0.01455772	0.71107595	1	0.25102192	1.06738195	6.48427572	0.03566893	0.01525927						
55	Ta_457P	Ta_457P	0.01391285	0.71392449	1	0.23512718	1.03213556	6.09544632	0.03468434	0.01497841						
56	Ta_4570	Ta_4570	0.41585167	2.50705121	1	0.14349953	0.79962807	12.9276304	0.08161144	0.03001929						
57	1a_45/N	Ta_45/N	5.0369939	27.3334103	, 1	0.38141528	0.96730066	25.4924805	0.38562893	0.19239971	_					



- 9. To the right of the "Master" section, there is another section which defines the base element. GO TO the column for your new matrix or "base" <u>AND</u> EDIT the cell over the line designation (SnKA1) formula to read, "If(xx=1000,"Base",""), where xx is the first cell in the matrix column below line designation (SnKA1). Frequently the formulas lose a reference and need to be retyped.
- 10. ADD and REMOVE the chemistry files and CREATE the chemistry calibration (see Section 7).

the new	chemi	stry index	:			WebEx Type a question for help ▼ - 6 OK % , % % 律 律 里 • ◊ • ▲ • .										
								J 5 85%	• 2	•		DU	01			
		_						_ <u>BD</u>	BE	BF	BG	BH	BI	BJ	BK	
								sKa1	PbLb1	BiLb1	ZrKa1	RhKa1	AgKat	SnKa1	SbKa1	
13	cu331	:11000-701	0.001	0.005	0.00							-				
4	cu332	17200-71	0.01	0.031	0.01	ld/Remove	Chemist	ry files				0				
5	cu333	31400-72B		0.01	0.00	PDZ Lis	t		-	Chemistry	/ List	0				
6	cu334	36000-731	0.001	0.17	0.05	al484				11331		0		0.15		
7	cu335	46400-741	0.01	0.011	0.00	al486				u332	-	0		0.5		
8	cu336	:48200-75	0.01	0.052	0.02	al487		Add		u333		0		0.89		
9	cu337	48500-76	0.01	0.08	0.0	al488			- (u334		0		0.99		
10	cu338	51000-77	0.01	0.01	0.0	al496				u335		0		4.6		
11	cu339	54400-781	0.005	0.02	0.0	al500		Unselec	t (cu336		0		4.35		
12	cu340	62300-79	0.25	2.2	0.23	4506				:u337		0				
13	cu341	63000-801	0.55	3.32	4.71	albeb 00170			- L2	:U338 W220		0		0.017		
14	cu342	64200-81	0.01	0.1	0.01	00171			e 2	-u339 -u340		0				
15	cu343	65500-82	1.02	0.04	0.0	co172	-	_	_ 2	10341	-	0				
16	cu344	67500-83	0.22	0.99	0.0							0		0.57		
17	cu345	70600-841	0.6	1.3	10			Add New Chamiata	íl 🗖	71.11	-	0				
18	cu346	71500-851	0.53	0.53	29.6			Criemisur		.01		0				
19	cu347	:83600-861	0.01	0.029	0.78							0		4.58	0.092	
20	cu348	:85700-87.	0.008	0.23	0.33	59.981	37.49		0.92	0	0	0		0.55	0.01	
21	cu349	86300-88	3.72	2.27	0.02	64.562	23.25		0.03	0	0	0				
22	cu350	90300-891	0.01	0.013	0.15	87.463	3.96		0.089	0	0	0		8.17		
23	cu351	92200-901	0.01	0.019	0.69	88.022	2.98		1.66	0	0	0		6.44	0.06	
24	cu352	93200-911	0.01	0.056	0.56	82	3.49		7.15	0	0	0		6.57	0.19	
25	cu353	93700-921	0.01	0.009	0.36	79.606	0.28		9.5	0	0	0		9.75	0.35	
26	cu354	95400-931	0.024	3.87	0.088	85.4	0.17		0.012	0	0	0		0.009		
27	cu355	95500-94	0.16	4.04	4.37	80.624	0.09		0.009	0	0	0	0			
28 C	U_WSB7	CU_WSB7	3.19	1.73	3.05	73.3	6.8	0.076	0.054	0			0	1.91	0.61	
29 0	Cu7134	Cu7134	0.05	0.29	0.01	87 168	1.55	0.18	2.47	0	0	0	0.025	8.2	0.01	

To add a 2nd or 3rd Chemistry "Cfz" to an existing matrix set--**SELECT** the Add/Remove Chem files", then **SELECT** at <u>least</u> 2 new PDZ files from the left column

SELECT "Add New Chemistry" and INSERT the next index number.





Appendix B Building a Flashcard Image

- 1. From the *Instrument Info* tab, open the S1 Cal Process menu.
- 2. **SELECT** Build PDA Image.
- 3. **RIGHT CLICK** in Grey area to **ADD** new Calibration Method/or Group.
- 4. **ENTER** the Method name that should appear on PDA for user selection.
- 5. **SELECT** the associated Sort and Chemistry files (*.srz and .CFZ).
- 6. If using "Compton" ratio method, **SELECT** the Compton (eV) range.

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