

How to Perform a Chemistry Analysis of Large Data Sets

- 1) **OPEN** the Excel calibration spread sheet for that material to be analyzed.
 - a) **SAVE** the sheet under a different name in the folder with your unknown data.
 - b) **KEEP** the original calibration sheet as an unaltered template.
- 2) **SELECT** the pdz tab in the spread sheet.
 - a) **CLICK** S1CALPROCESS.
 - b) **SELECT** the Insert PDZ option in the drop down.
- 3) **FIND** and **HIGHLIGHT** the spectra you want analyzed and **INSERT** them.
- 4) **SCROLL DOWN** to where the names appear and **HIGHLIGHT** them. The names are in Column B.
- 5) **COPY** the names.
- 6) **SELECT** the Chem Tests Tab at the bottom of the Excel page.
- 7) **PASTE** the names in Column F. 
- 8) In column G, **TYPE** in the calibration file name (e.g., GL1, or CU1). **DO NOT INCLUDE FILE EXTENSION.**
 - a) **ENSURE** the names extend all the way down by each spectra name.
 - b) (**Note:** the CFZ calibration file is saved in the folder listed on the Instrument info tab in cell F1. The Chem Test macro will use  GL1 or CU1 coefficients directly from the Calibration spreadsheet.)
- 9) **SELECT** the Chem Test tab in the S1Calprocess drop down and **ENSURE** all spectral files are listed in the window.
- 10) **DOUBLE CLICK** on any spectra file listed to analyze all files in the Window. It immediately produces an analysis table of all the samples for each element and puts the values in the spread sheet next to each of the spectra and element names.
- 11) **COPY** and **PASTE** the data file names to the column in front of the table of values.
- 12) **COPY** and **PASTE** the element names to the top of the table.
- 13) **COPY** this entire table of names, elements and values to a separate spread sheet. The values are in whatever units used to do the calibration.
- 14) Questions? **CONTACT** Bruker.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	C:\Documents and Settings\ferguson\Desktop\8-18-08 obs cal													
2		AKC008_t1	AKC008_t1	GI1	180.09	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
3		AKC008_t2	AKC008_t2	GI1	180.09	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
4		AKC008_t3	AKC008_t3	GI1	180.97	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
5		ALCA1_T1	ALCA1_T1	GI1	180.15	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
6		ALCA1_t2	ALCA1_t2	GI1	180.12	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
7		ALCA1_t3	ALCA1_t3	GI1	180.12	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
8		ANCA10_t1	ANCA10_t1	GI1	180.1	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
9		ANCA10_t2	ANCA10_t2	GI1	180.06	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
10		ANCA10_t3	ANCA10_t3	GI1	180.05	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
11		BARD09_t1	BARD09_t1	GI1	180.07	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
12		BARD09_t2	BARD09_t2	GI1	180.09	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
13		BARD09_t3	BARD09_t3	GI1	180.16	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
14		BGID01_t1	BGID01_t1	GI1	180.12	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
15		BGID01_t2	BGID01_t2	GI1	180.1	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
16		BGID01_t3	BGID01_t3	GI1	180.09	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
17		BLCA04_t1	BLCA04_t1	GI1	180.06	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			
18		BLCA04_t2	BLCA04_t2	GI1	180.1	NaKa1	AlKa1	K Ka1	BaLa1	TiKa1	MnKa1			

 PDZ file name
(copied from PDZ sheet)
  Cal file name
  Elements of interest