ICP-MS Data Processing Software from Robinson Scientific Ltd

About us

Gavin Robinson has almost 20 years experience with ICP-MS instruments and data processing, including 14 years at Hill Laboratories in Hamilton, New Zealand (the largest privately owned commercial testing lab in the country), where Gav was a senior manager and shareholder, with responsibilities including managing the Trace Elements testing section, and implementing LIMS data integration lab-wide.

Gav has operated and serviced VG (now Thermo) and PerkinElmer ICP-MS instruments for many years, and is the NZ distributor for PerkinElmer ICP-MS instruments.

Robinson Scientific are experts at designing and implementing all manner of systems for laboratories. We also excel with data processing software and systems.

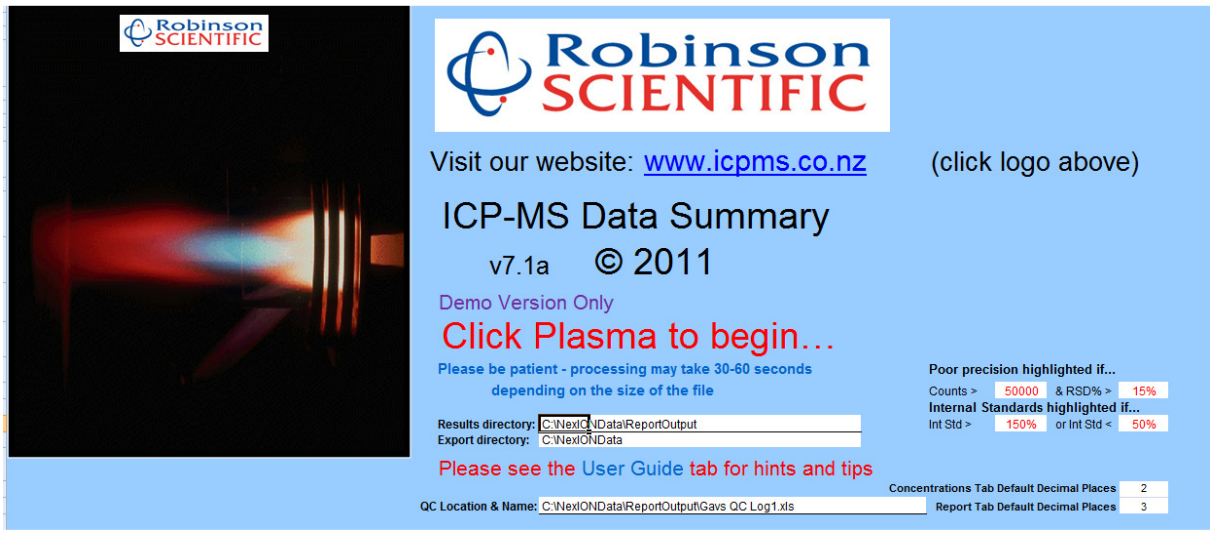
ICP-MS Data Processing Software

We know what to look for when appraising ICP-MS data, and have developed smart spreadsheet software over the years to make the operators life easier and improve efficiencies, as well as reducing the potential for human or typographical data transfer errors.

Our software is available for sale from info@icpms.co.nz
or visit our web site: www.icpms.co.nz

ICP-MS data processing software programming code is VBA, user interface is Excel. We recommend Excel 2007 or later to ensure best functionality, although the software will usually work OK with earlier versions.

Main screen:



Notes & Comments from the User Guide:

- Once loaded into Excel using this software tool, the data can be manipulated as desired using normal Excel functions – we can also 'lock' the data if desired so it cannot be altered accidentally.

- The file format is important as the software looks for certain symbols such as "|>" to indicate an isotope is an internal standard. Also the order of columns and header rows is important to ensure data is imported correctly.

- Please use the Report Options file provided by Robinson Scientific Ltd

- If you have specific reasons for needing to use a different Report Options file please contact us and we may be able to customise the software to accommodate this.

- **Note:** macros need to be enabled (under security settings) for the coding to be able to work.

- Internal Standard cells will be highlighted (red text) when the values are outside the ranges specified on the main page.

- Cells will automatically be highlighted (in green) when they fall outside the precision criteria defined on the front page of this program

- Rows will automatically be highlighted when the word "BLANK" is found in the Sample ID.

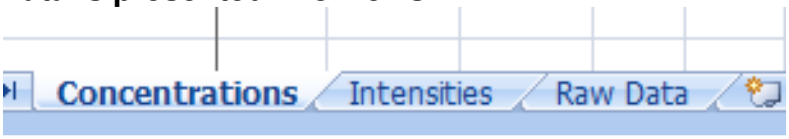
- The default Results Directory can be altered and the program saved with this changed.

- **To re-load the file you are viewing, simply click on the "Re-load" button which is located at the top left on the Concentrations tab**
  (NB: Main Data Summary program must still be open)

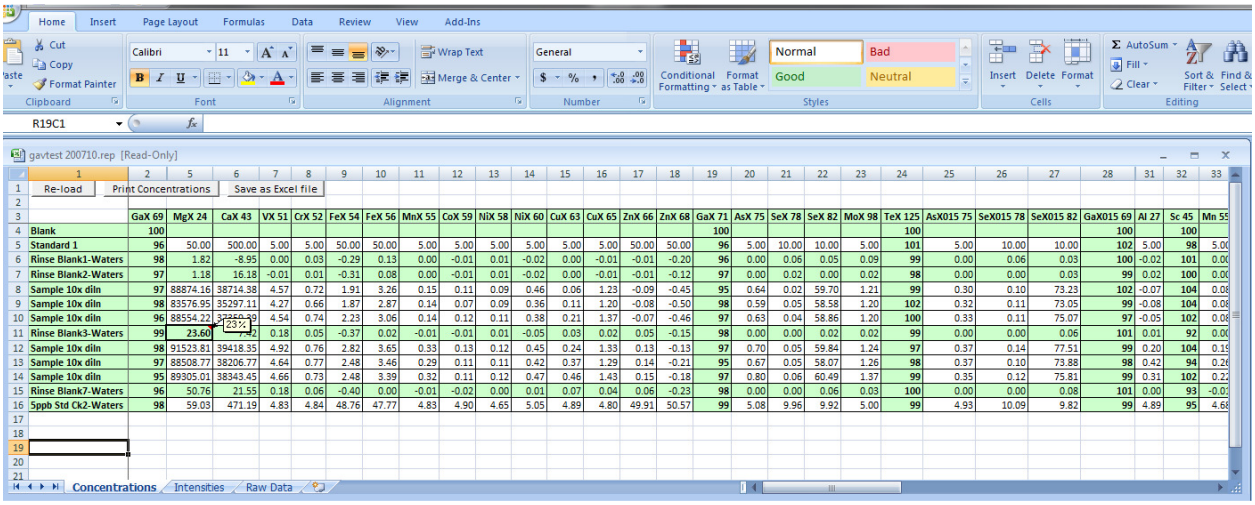
- To see the RSD for any samples highlighted outside your set precision range simply hover the cursor over those cells

- A high degree of customisation is available – please contact us to discuss your requirements. We can help integrate with your LIMS – price on request

Data is presented in 3 views:



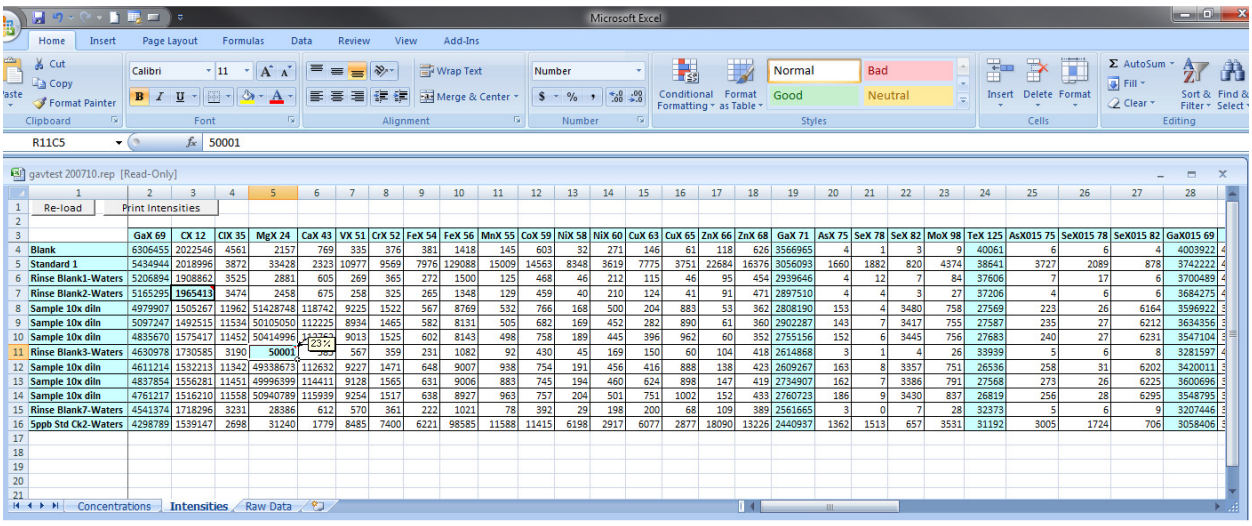
Concentrations View:



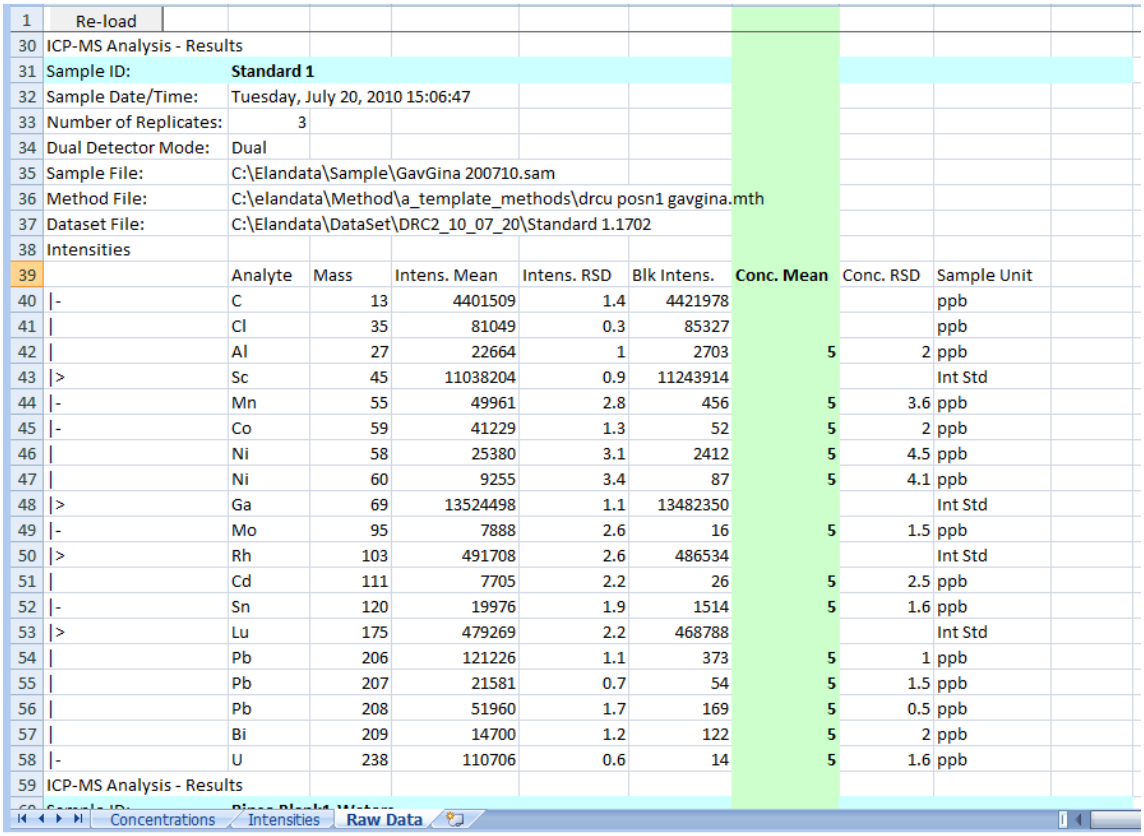
Note the highlighted poor precision – in this case due to carry-over from a high sample:

9	Sample 10x diln	98	83576.95	35297.11	4.27	0.66
10	Sample 10x diln	96	88554.22	[illegible]	4.54	0.74
11	Rinse Blank3-Waters	99	23.60	[illegible]	0.18	0.05
12	Sample 10x diln	98	91523.81	39418.35	4.92	0.76
13	Sample 10x diln	97	88508.77	38206.77	4.64	0.77
14	Sample 10x diln	95	89305.01	38343.45	4.66	0.73
15	Rinse Blank7-Waters	96	50.76	21.55	0.18	0.06
16	5ppb Std Ck2-Waters	98	59.03	471.19	4.83	4.84

Intensities View (shows counts per second):



Raw Data View: (this is very similar to the normal Elan / NexION printout):



1	Re-load							
30	ICP-MS Analysis - Results							
31	Sample ID:	**Standard 1**						
32	Sample Date/Time:	Tuesday, July 20, 2010 15:06:47						
33	Number of Replicates:	3						
34	Dual Detector Mode:	Dual						
35	Sample File:	C:\Elandata\Sample\GavGina 200710.sam						
36	Method File:	C:\elandata\Method\a_template_methods\drcu posn1 gavgina.mth						
37	Dataset File:	C:\Elandata\DataSet\DRC2_10_07_20\Standard 1.1702						
38	Intensities							
39		Analyte	Mass	Intens. Mean	Intens. RSD	Blk Intens.	**Conc. Mean**	Conc. RSD	Sample Unit
40	|-	C	13	4401509	1.4	4421978			ppb
41	|	Cl	35	81049	0.3	85327			ppb
42	|	Al	27	22664	1	2703	5	2	ppb
43	|>	Sc	45	11038204	0.9	11243914			Int Std
44	|-	Mn	55	49961	2.8	456	5	3.6	ppb
45	|-	Co	59	41229	1.3	52	5	2	ppb
46	|	Ni	58	25380	3.1	2412	5	4.5	ppb
47	|	Ni	60	9255	3.4	87	5	4.1	ppb
48	|>	Ga	69	13524498	1.1	13482350			Int Std
49	|-	Mo	95	7888	2.6	16	5	1.5	ppb
50	|>	Rh	103	491708	2.6	486534			Int Std
51	|	Cd	111	7705	2.2	26	5	2.5	ppb
52	|-	Sn	120	19976	1.9	1514	5	1.6	ppb
53	|>	Lu	175	479269	2.2	468788			Int Std
54	|	Pb	206	121226	1.1	373	5	1	ppb
55	|	Pb	207	21581	0.7	54	5	1.5	ppb
56	|	Pb	208	51960	1.7	169	5	0.5	ppb
57	|	Bi	209	14700	1.2	122	5	2	ppb
58	|-	U	238	110706	0.6	14	5	1.6	ppb
59	ICP-MS Analysis - Results								

Concentrations | Intensities | Raw Data

Summary of Standard Features:

- Easy viewing of data as it is being acquired, plus one-button ‘Re-Load’
- Concentrations, Intensities (cps) and Raw Data (like normal printout) viewable
- User defined number of decimal places
- Internal Standards highlighted if outside your user defined ranges
- Poor precision highlighted if outside your user defined parameters
- User defined file directories

Summary of Advanced Features (available after clicking “Go To Processing”:

- Blank subtraction
- Automatic averaging of data (rows)
- Multiply by dilution factors (preparation and analysis dilution steps)
- Conversion (e.g. from ppb to ppm) – user defined conversion factor
- Drift correction (e.g. to correct for any drift present)
- Baseline correction (to correct for memory effects, washout etc)
- Audit Trail for drift and baseline correction
- User defined detection limits (3 levels)
- User defined significant figures (for results and detection limits)
- Automatic spike recovery calculations
- Show / Hide isotopes of interest
- Automatic QC logging (to a user defined QC log and directory)
- OPTION: an export file can be generated for your LIMS system at the click of a button

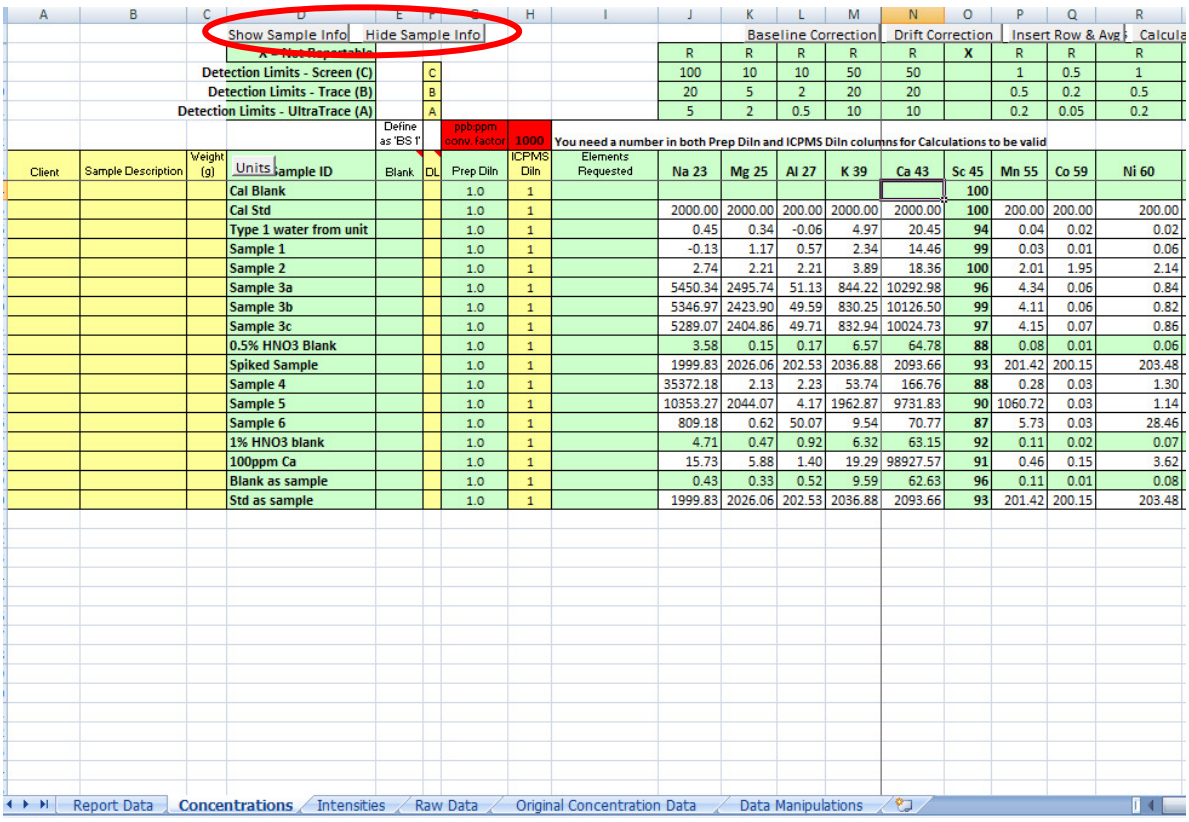
Details for Advanced Features (available after clicking "Go To Processing":

(note when clicking on this, your **original** Concentration data is saved on a separate tab, named "**Original Concentration Data**" – this is to ensure the original data is always available, even after you perform manipulations on the **Concentration** data).

Show / Hide Sample Information

On the **Concentrations** tab or **Report Data** tab of the spreadsheet, the sample information (e.g. columns A-C and E-I) can be hidden (it is shown by default) by clicking the **Hide Sample Info** button, or shown again by clicking the **Show Sample Info** button.

Example – all info shown (as is the default):



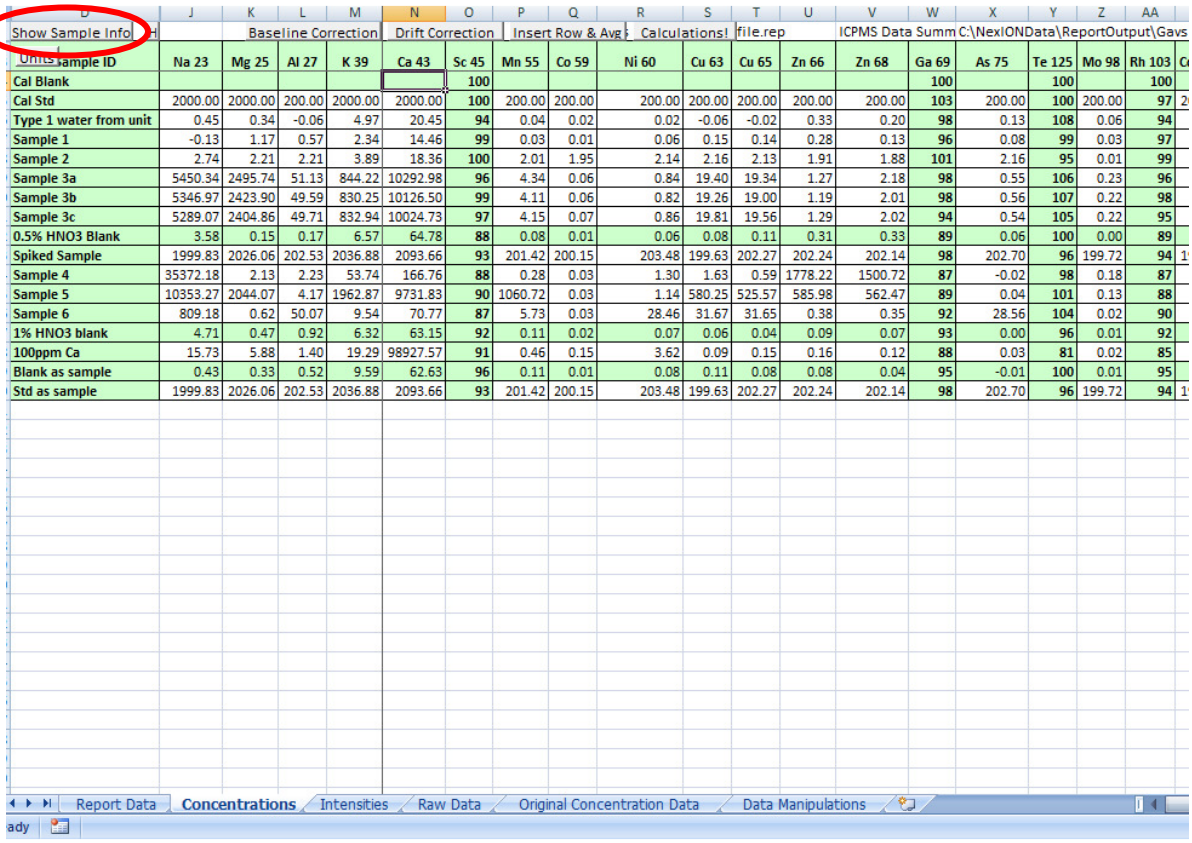
Show Sample Info | Hide Sample Info

													Baseline Correction				Drift Correction		Insert Row & Avg		Calcula		
			A = Not Reportable										R	R	R	R	R	X	R	R	R		
			Detection Limits - Screen (C)		C								100	10	10	50	50		1	0.5	1		
			Detection Limits - Trace (B)		B								20	5	2	20	20		0.5	0.2	0.5		
			Detection Limits - UltraTrace (A)		A								5	2	0.5	10	10		0.2	0.05	0.2		
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns for Calculations to be valid															
Client	Sample Description	Weight (g)	Units / Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested	Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45	Mn 55	Co 59	Ni 60						
			Cal Blank			1.0	1							100									
			Cal Std			1.0	1		2000.00	2000.00	200.00	2000.00	2000.00	100	200.00	200.00	200.00						
			Type 1 water from unit			1.0	1		0.45	0.34	-0.06	4.97	20.45	94	0.04	0.02	0.02						
			Sample 1			1.0	1		-0.13	1.17	0.57	2.34	14.46	99	0.03	0.01	0.06						
			Sample 2			1.0	1		2.74	2.21	2.21	3.89	18.36	100	2.01	1.95	2.14						
			Sample 3a			1.0	1		5450.34	2495.74	51.13	844.22	10292.98	96	4.34	0.06	0.84						
			Sample 3b			1.0	1		5346.97	2423.90	49.59	830.25	10126.50	99	4.11	0.06	0.82						
			Sample 3c			1.0	1		5289.07	2404.86	49.71	832.94	10024.73	97	4.15	0.07	0.86						
			0.5% HNO3 Blank			1.0	1		3.58	0.15	0.17	6.57	64.78	88	0.08	0.01	0.06						
			Spiked Sample			1.0	1		1999.83	2026.06	202.53	2036.88	2093.66	93	201.42	200.15	203.48						
			Sample 4			1.0	1		35372.18	2.13	2.23	53.74	166.76	88	0.28	0.03	1.30						
			Sample 5			1.0	1		10353.27	2044.07	4.17	1962.87	9731.83	90	1060.72	0.03	1.14						
			Sample 6			1.0	1		809.18	0.62	50.07	9.54	70.77	87	5.73	0.03	28.46						
			1% HNO3 blank			1.0	1		4.71	0.47	0.92	6.32	63.15	92	0.11	0.02	0.07						
			100ppm Ca			1.0	1		15.73	5.88	1.40	19.29	98927.57	91	0.46	0.15	3.62						
			Blank as sample			1.0	1		0.43	0.33	0.52	9.59	62.63	96	0.11	0.01	0.08						
			Std as sample			1.0	1		1999.83	2026.06	202.53	2036.88	2093.66	93	201.42	200.15	203.48						

Report Data | Concentrations | Intensities | Raw Data | Original Concentration Data | Data Manipulations

[Please see next page]

Example – sample information hidden – to unhide click Show Sample Info button:



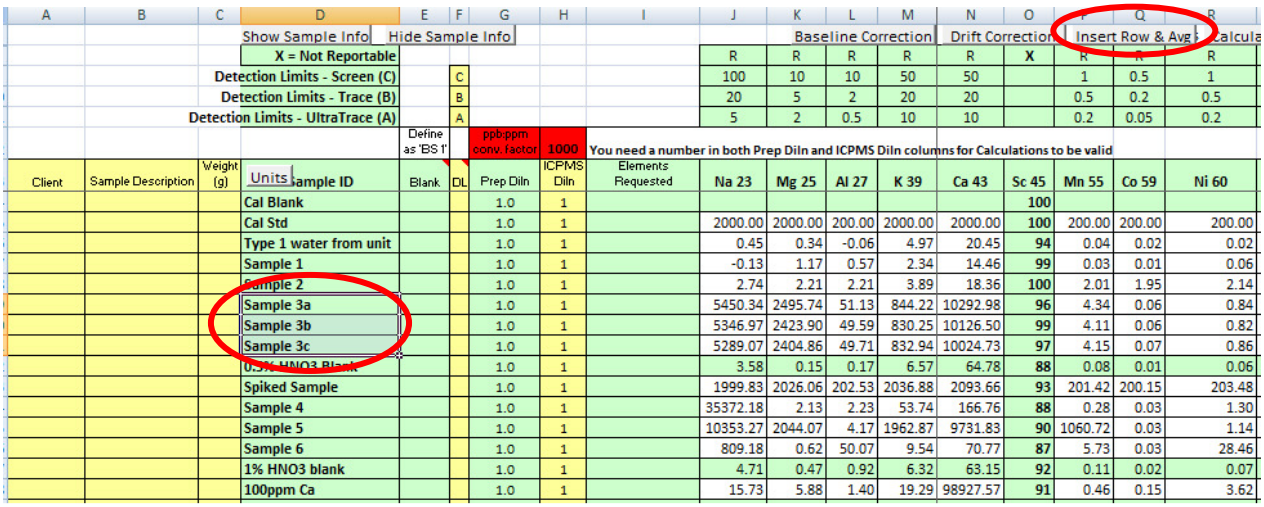
Show Sample Info		Baseline Correction			Drift Correction	Insert Row & Avg		Calculations!	file.rep			ICPMS Data Summ	C:\NexIONData\ReportOutput\Gavs				
Units / Sample ID	Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45	Mn 55	Co 59	Ni 60	Cu 63	Cu 65	Zn 66	Zn 68	Ga 69	As 75	Te 125	Mo 98	Rh 103
Cal Blank						100								100		100		100
Cal Std	2000.00	2000.00	200.00	2000.00	2000.00	100	200.00	200.00	200.00	200.00	200.00	200.00	200.00	103	200.00	100	200.00	97
Type 1 water from unit	0.45	0.34	-0.06	4.97	20.45	94	0.04	0.02	0.02	-0.06	-0.02	0.33	0.20	98	0.13	108	0.06	94
Sample 1	-0.13	1.17	0.57	2.34	14.46	99	0.03	0.01	0.06	0.15	0.14	0.28	0.13	96	0.08	99	0.03	97
Sample 2	2.74	2.21	2.21	3.89	18.36	100	2.01	1.95	2.14	2.16	2.13	1.91	1.88	101	2.16	95	0.01	99
Sample 3a	5450.34	2495.74	51.13	844.22	10292.98	96	4.34	0.06	0.84	19.40	19.34	1.27	2.18	98	0.55	106	0.23	96
Sample 3b	5346.97	2423.90	49.59	830.25	10126.50	99	4.11	0.06	0.82	19.26	19.00	1.19	2.01	98	0.56	107	0.22	98
Sample 3c	5289.07	2404.86	49.71	832.94	10024.73	97	4.15	0.07	0.86	19.81	19.56	1.29	2.02	94	0.54	105	0.22	95
0.5% HNO3 Blank	3.58	0.15	0.17	6.57	64.78	88	0.08	0.01	0.06	0.08	0.11	0.31	0.33	89	0.06	100	0.00	89
Spiked Sample	1999.83	2026.06	202.53	2036.88	2093.66	93	201.42	200.15	203.48	199.63	202.27	202.24	202.14	98	202.70	96	199.72	94
Sample 4	35372.18	2.13	2.23	53.74	166.76	88	0.28	0.03	1.30	1.63	0.59	1778.22	1500.72	87	-0.02	98	0.18	87
Sample 5	10353.27	2044.07	4.17	1962.87	9731.83	90	1060.72	0.03	1.14	580.25	525.57	585.98	562.47	89	0.04	101	0.13	88
Sample 6	809.18	0.62	50.07	9.54	70.77	87	5.73	0.03	28.46	31.67	31.65	0.38	0.35	92	28.56	104	0.02	90
1% HNO3 blank	4.71	0.47	0.92	6.32	63.15	92	0.11	0.02	0.07	0.06	0.04	0.09	0.07	93	0.00	96	0.01	92
100ppm Ca	15.73	5.88	1.40	19.29	98927.57	91	0.46	0.15	3.62	0.09	0.15	0.16	0.12	88	0.03	81	0.02	85
Blank as sample	0.43	0.33	0.52	9.59	62.63	96	0.11	0.01	0.08	0.11	0.08	0.08	0.04	95	-0.01	100	0.01	95
Std as sample	1999.83	2026.06	202.53	2036.88	2093.66	93	201.42	200.15	203.48	199.63	202.27	202.24	202.14	98	202.70	96	199.72	94

Report Data | Concentrations | Intensities | Raw Data | Original Concentration Data | Data Manipulations

Automatic Averaging of Data

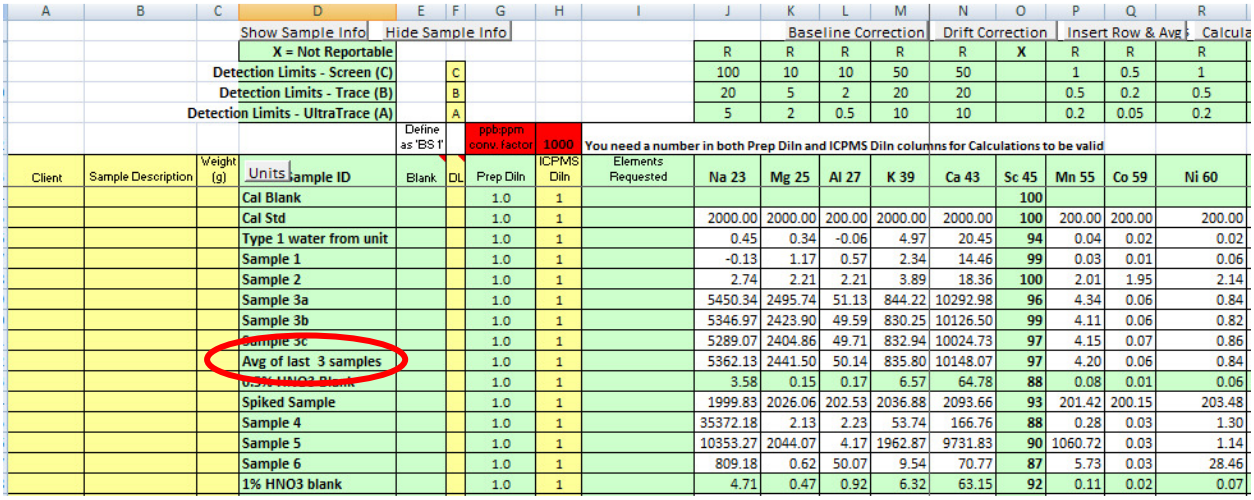
Samples (rows of data) can be automatically averaged, simply by highlighting the Sample ID for the rows you want to average, then clicking on the Insert Row & Avg button. See example below. Once averaged, the average sample may be named anything you like.

Example – averaging triplicate samples:



			Show Sample Info	Hide Sample Info						Baseline Correction				Drift Correction		Insert Row & Avg		
			X = Not Reportable							R	R	R	R	R	X	R	R	R
			Detection Limits - Screen (C)		C					100	10	10	50	50		1	0.5	1
			Detection Limits - Trace (B)		B					20	5	2	20	20		0.5	0.2	0.5
			Detection Limits - UltraTrace (A)		A					5	2	0.5	10	10		0.2	0.05	0.2
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns for Calculations to be valid										
Client	Sample Description	Weight (g)	Units / Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested	Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45	Mn 55	Co 59	Ni 60	
			Cal Blank			1.0	1							100				
			Cal Std			1.0	1		2000.00	2000.00	200.00	2000.00	2000.00	100	200.00	200.00	200.00	
			Type 1 water from unit			1.0	1		0.45	0.34	-0.06	4.97	20.45	94	0.04	0.02	0.02	
			Sample 1			1.0	1		-0.13	1.17	0.57	2.34	14.46	99	0.03	0.01	0.06	
			Sample 2			1.0	1		2.74	2.21	2.21	3.89	18.36	100	2.01	1.95	2.14	
			Sample 3a			1.0	1		5450.34	2495.74	51.13	844.22	10292.98	96	4.34	0.06	0.84	
			Sample 3b			1.0	1		5346.97	2423.90	49.59	830.25	10126.50	99	4.11	0.06	0.82	
			Sample 3c			1.0	1		5289.07	2404.86	49.71	832.94	10024.73	97	4.15	0.07	0.86	
			0.5% HNO3 Blank			1.0	1		3.58	0.15	0.17	6.57	64.78	88	0.08	0.01	0.06	
			Spiked Sample			1.0	1		1999.83	2026.06	202.53	2036.88	2093.66	93	201.42	200.15	203.48	
			Sample 4			1.0	1		35372.18	2.13	2.23	53.74	166.76	88	0.28	0.03	1.30	
			Sample 5			1.0	1		10353.27	2044.07	4.17	1962.87	9731.83	90	1060.72	0.03	1.14	
			Sample 6			1.0	1		809.18	0.62	50.07	9.54	70.77	87	5.73	0.03	28.46	
			1% HNO3 blank			1.0	1		4.71	0.47	0.92	6.32	63.15	92	0.11	0.02	0.07	
			100ppm Ca			1.0	1		15.73	5.88	1.40	19.29	98927.57	91	0.46	0.15	3.62	

Automatic averaging of data - here's the result:



			Show Sample Info	Hide Sample Info							Baseline Correction				Drift Correction		Insert Row & Avg		Calcula	
			X = Not Reportable							R	R	R	R	R	X	R	R	R		
			Detection Limits - Screen (C)		C					100	10	10	50	50		1	0.5	1		
			Detection Limits - Trace (B)		B					20	5	2	20	20		0.5	0.2	0.5		
			Detection Limits - UltraTrace (A)		A					5	2	0.5	10	10		0.2	0.05	0.2		
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns for Calculations to be valid												
Client	Sample Description	Weight (g)	Units Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested	Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45	Mn 55	Co 59	Ni 60			
			Cal Blank			1.0	1							100						
			Cal Std			1.0	1		2000.00	2000.00	200.00	2000.00	2000.00	100	200.00	200.00	200.00			
			Type 1 water from unit			1.0	1		0.45	0.34	-0.06	4.97	20.45	94	0.04	0.02	0.02			
			Sample 1			1.0	1		-0.13	1.17	0.57	2.34	14.46	99	0.03	0.01	0.06			
			Sample 2			1.0	1		2.74	2.21	2.21	3.89	18.36	100	2.01	1.95	2.14			
			Sample 3a			1.0	1		5450.34	2495.74	51.13	844.22	10292.98	96	4.34	0.06	0.84			
			Sample 3b			1.0	1		5346.97	2423.90	49.59	830.25	10126.50	99	4.11	0.06	0.82			
			Sample 3c			1.0	1		5289.07	2404.86	49.71	832.94	10024.73	97	4.15	0.07	0.86			
			Avg of last 3 samples			1.0	1		5362.13	2441.50	50.14	835.80	10148.07	97	4.20	0.06	0.84			
			0.5% HNO3 Blank			1.0	1		3.58	0.15	0.17	6.57	64.78	88	0.08	0.01	0.06			
			Spiked Sample			1.0	1		1999.83	2026.06	202.53	2036.88	2093.66	93	201.42	200.15	203.48			
			Sample 4			1.0	1		35372.18	2.13	2.23	53.74	166.76	88	0.28	0.03	1.30			
			Sample 5			1.0	1		10353.27	2044.07	4.17	1962.87	9731.83	90	1060.72	0.03	1.14			
			Sample 6			1.0	1		809.18	0.62	50.07	9.54	70.77	87	5.73	0.03	28.46			
			1% HNO3 blank			1.0	1		4.71	0.47	0.92	6.32	63.15	92	0.11	0.02	0.07			

Blank subtraction

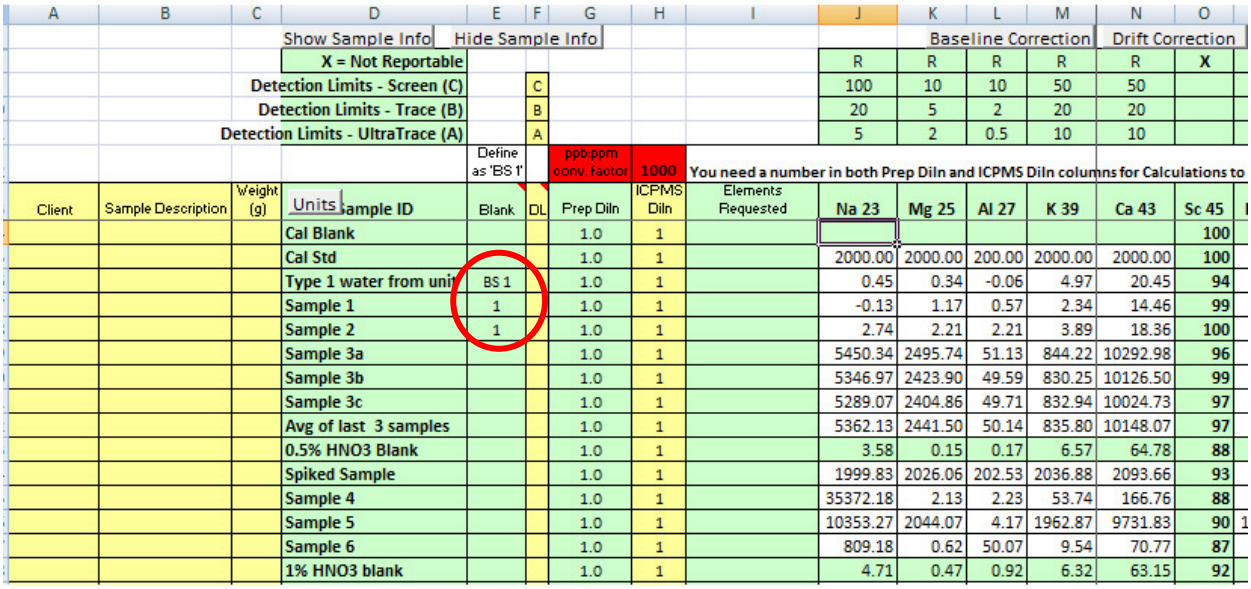
In the Blank column, enter "BS 1" (without the quotes) to define a sample as Blank 1. Then enter "1" (without the quotes) in the Blank column for all samples you wish to subtract this blank from.

You may have up to different 30 blanks defined to be subtracted.

Blanks will be subtracted when you click on the **Calculations!** Button (top mid-right of the screen on the Concentrations Tab).

Blank subtracted data is displayed on the **Report Data** tab.

Example – subtracting blanks:



			Show Sample Info	Hide Sample Info							Baseline Correction				Drift Correction	
			X = Not Reportable							R	R	R	R	R	X	
			Detection Limits - Screen (C)		C					100	10	10	50	50		
			Detection Limits - Trace (B)		B					20	5	2	20	20		
			Detection Limits - UltraTrace (A)		A					5	2	0.5	10	10		
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns for Calculations to								
Client	Sample Description	Weight (g)	Units Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested	Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45		
			Cal Blank			1.0	1							100		
			Cal Std			1.0	1		2000.00	2000.00	200.00	2000.00	2000.00	100		
			Type 1 water from unit	BS 1		1.0	1		0.45	0.34	-0.06	4.97	20.45	94		
			Sample 1	1		1.0	1		-0.13	1.17	0.57	2.34	14.46	99		
			Sample 2	1		1.0	1		2.74	2.21	2.21	3.89	18.36	100		
			Sample 3a			1.0	1		5450.34	2495.74	51.13	844.22	10292.98	96		
			Sample 3b			1.0	1		5346.97	2423.90	49.59	830.25	10126.50	99		
			Sample 3c			1.0	1		5289.07	2404.86	49.71	832.94	10024.73	97		
			Avg of last 3 samples			1.0	1		5362.13	2441.50	50.14	835.80	10148.07	97		
			0.5% HNO3 Blank			1.0	1		3.58	0.15	0.17	6.57	64.78	88		
			Spiked Sample			1.0	1		1999.83	2026.06	202.53	2036.88	2093.66	93		
			Sample 4			1.0	1		35372.18	2.13	2.23	53.74	166.76	88		
			Sample 5			1.0	1		10353.27	2044.07	4.17	1962.87	9731.83	90		
			Sample 6			1.0	1		809.18	0.62	50.07	9.54	70.77	87		
			1% HNO3 blank			1.0	1		4.71	0.47	0.92	6.32	63.15	92		

Multiply by dilution factors

Dilution factors can be entered in the “ICPMS Diln” and “Prep Diln” columns.

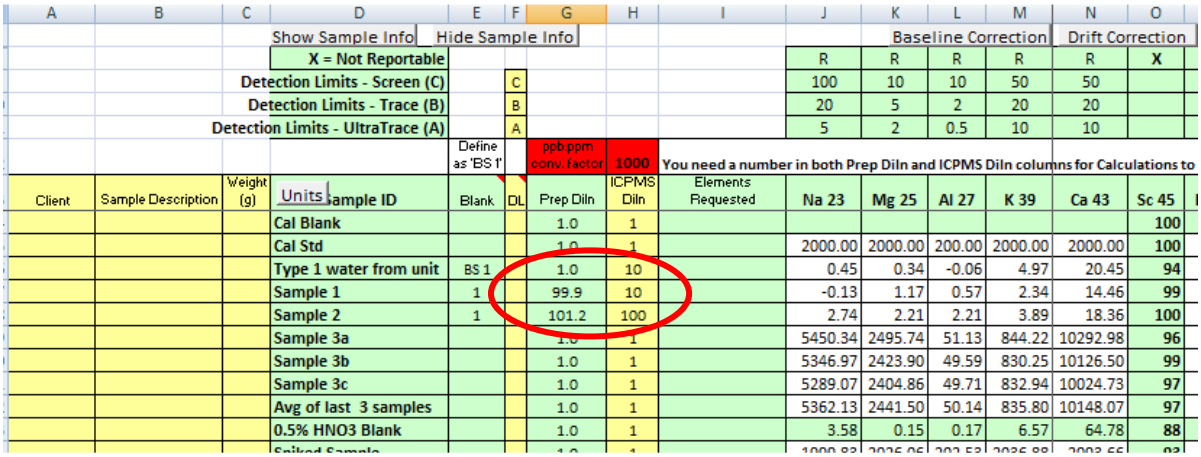
ICPMS dilution refers to the dilution immediately prior to analysis, e.g. if a digest or extract was diluted say 10x prior to analysis.

Prep dilution refers to the dilution as part of the sample preparation procedure, e.g. 0.5g sample weighed out, digested and made to 50mL would be a Prep Dilution of 100x.

Data corrected for dilution factors is displayed on the **Report Data** tab.

Please note: you need a number (can be 1) in both Prep Diln and ICPMS Diln columns for the calculations to be valid (otherwise the conc gets multiplied by zero).

Example – multiplying by dilution factors:



			Show Sample Info	Hide Sample Info							Baseline Correction				Drift Correction		
			X = Not Reportable							R	R	R	R	R	X		
			Detection Limits - Screen (C)		C					100	10	10	50	50			
			Detection Limits - Trace (B)		B					20	5	2	20	20			
			Detection Limits - UltraTrace (A)		A					5	2	0.5	10	10			
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns for Calculations to									
Client	Sample Description	Weight (g)	Units Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested		Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45		
			Cal Blank			1.0	1								100		
			Cal Std			1.0	1			2000.00	2000.00	200.00	2000.00	2000.00	100		
			Type 1 water from unit	BS 1		1.0	10			0.45	0.34	-0.06	4.97	20.45	94		
			Sample 1	1		99.9	10			-0.13	1.17	0.57	2.34	14.46	99		
			Sample 2	1		101.2	100			2.74	2.21	2.21	3.89	18.36	100		
			Sample 3a			1.0	1			5450.34	2495.74	51.13	844.22	10292.98	96		
			Sample 3b			1.0	1			5346.97	2423.90	49.59	830.25	10126.50	99		
			Sample 3c			1.0	1			5289.07	2404.86	49.71	832.94	10024.73	97		
			Avg of last 3 samples			1.0	1			5362.13	2441.50	50.14	835.80	10148.07	97		
			0.5% HNO3 Blank			1.0	1			3.58	0.15	0.17	6.57	64.78	88		

Calculation Order

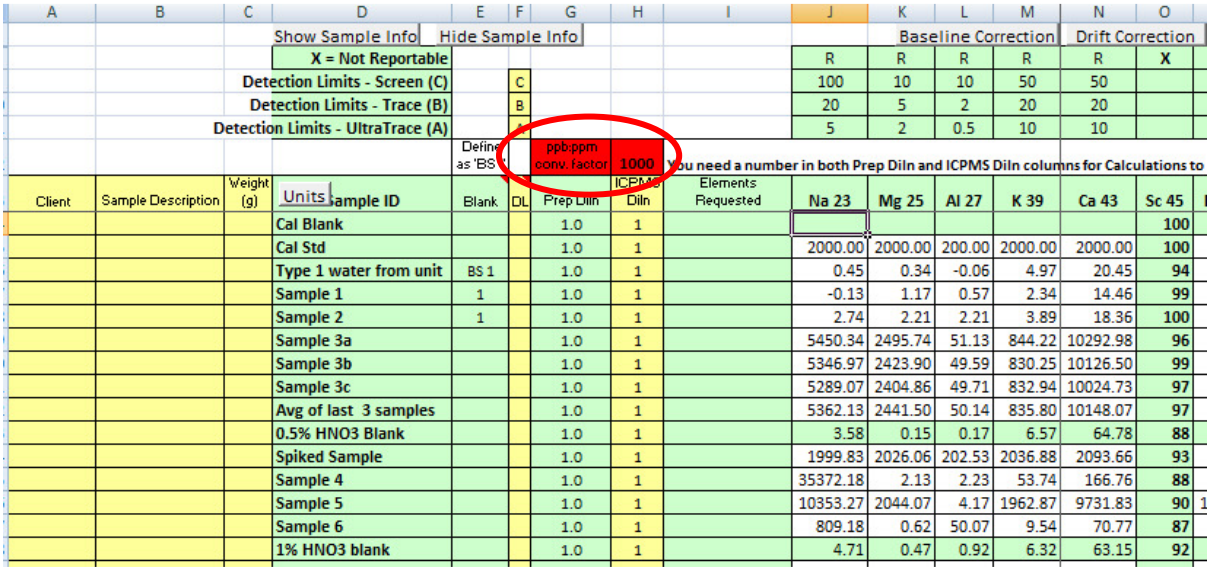
The order calculations are performed is:

([Sample Conc] **x** [ICPMS Diln]) **–** ([Assigned Blank (if any)] **x** [it’s ICPMS Diln]) **x** [Prep Diln]

Conversion (e.g. from ppb to ppm)”

All concentrations on the **Concentrations** tab can be converted from results displayed (often in ppb) to results to report (often ppm) on the **Report Data** tab, using the “ppb:ppm con.v factor” cell. By default this is set to 1000, to convert ppb to ppm, but it can be set to any value. Set this to “1” if you don’t want to convert the data by a factor.

Example – conversion factor:



			Show Sample Info	Hide Sample Info							Baseline Correction				Drift Correction	
			X = Not Reportable							R	R	R	R	R	X	
			Detection Limits - Screen (C)		C					100	10	10	50	50		
			Detection Limits - Trace (B)		B					20	5	2	20	20		
			Detection Limits - UltraTrace (A)		A					5	2	0.5	10	10		
				Define as 'BS'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns for Calculations to								
Client	Sample Description	Weight (g)	Units Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested		Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45	
			Cal Blank			1.0	1								100	
			Cal Std			1.0	1			2000.00	2000.00	200.00	2000.00	2000.00	100	
			Type 1 water from unit	BS 1		1.0	1			0.45	0.34	-0.06	4.97	20.45	94	
			Sample 1	1		1.0	1			-0.13	1.17	0.57	2.34	14.46	99	
			Sample 2	1		1.0	1			2.74	2.21	2.21	3.89	18.36	100	
			Sample 3a			1.0	1			5450.34	2495.74	51.13	844.22	10292.98	96	
			Sample 3b			1.0	1			5346.97	2423.90	49.59	830.25	10126.50	99	
			Sample 3c			1.0	1			5289.07	2404.86	49.71	832.94	10024.73	97	
			Avg of last 3 samples			1.0	1			5362.13	2441.50	50.14	835.80	10148.07	97	
			0.5% HNO3 Blank			1.0	1			3.58	0.15	0.17	6.57	64.78	88	
			Spiked Sample			1.0	1			1999.83	2026.06	202.53	2036.88	2093.66	93	
			Sample 4			1.0	1			35372.18	2.13	2.23	53.74	166.76	88	
			Sample 5			1.0	1			10353.27	2044.07	4.17	1962.87	9731.83	90	
			Sample 6			1.0	1			809.18	0.62	50.07	9.54	70.77	87	
			1% HNO3 blank			1.0	1			4.71	0.47	0.92	6.32	63.15	92	

Drift Correction

In any cases where drift has occurred in the analysis run, for example the 100ppb standard has been read back at say 110ppb, the data can be automatically Drift Corrected, which increments the correction from the start to the end of the data highlighted.

Please note: only one column can be corrected at a time. You must be on the **Concentrations** tab to perform drift or baseline corrections.

Note for Drift and Baseline Corrections: any corrections that are performed are automatically audit trailed – in other words a time and date stamped record is stored on the Data Manipulations tab of the spreadsheet.

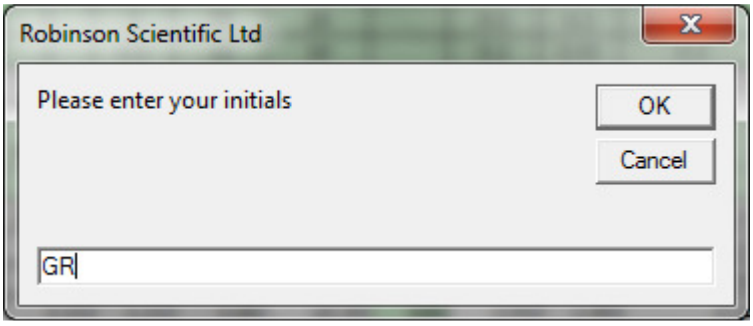
Terminology: **Blanket correction** means apply the same correction to the whole block of highlighted data, e.g. to correct a block of data up or down the same amount from start to finish. **Drift correction** allows you to define the start and end values to correct by.

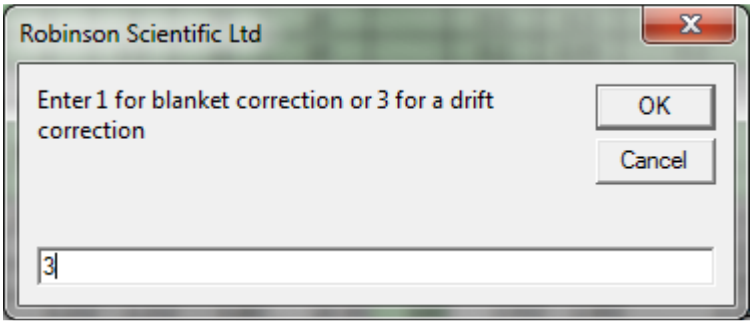
Procedure: on the **Concentrations** tab, simply highlight the data you wish to correct (one row at a time), then click on the Drift Correction button and follow the prompts.

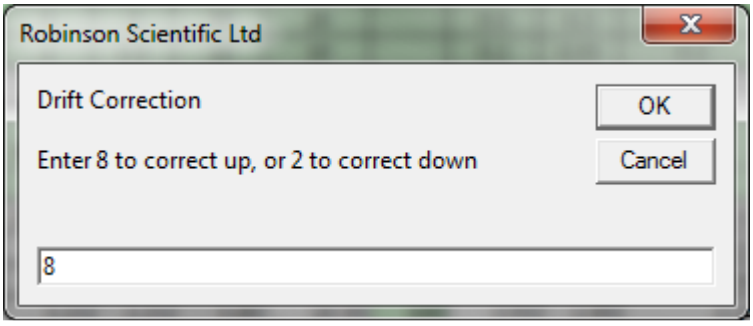
[Please see next page]

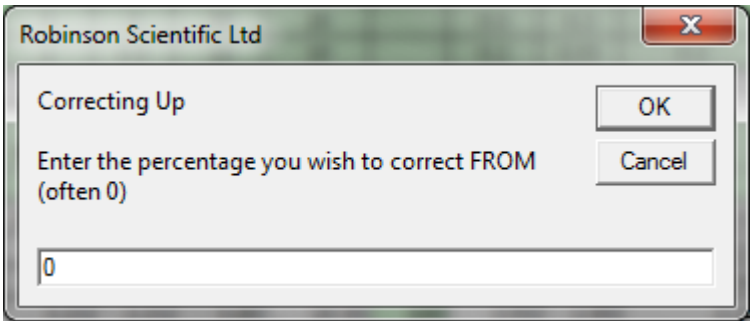
Example – drift correction - in this case the 200ppb standard for Pb 206 is reading 187ppb at the end of the run, so we wish to drift correct it UP 6.5% from the calibrating standard to the standard check at the end of the run:

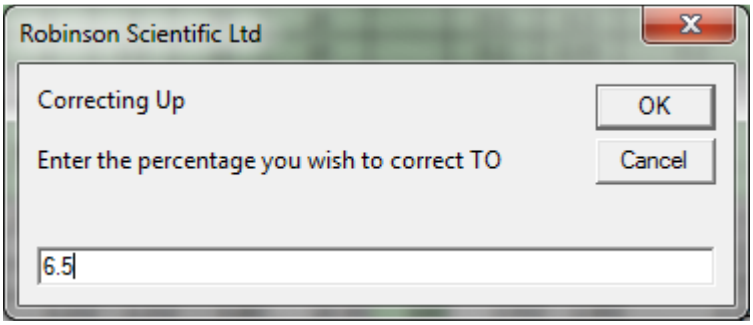
	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	AF	AG	AH
	Show Sample Info	Hide Sample Info								Baseline Correction	Drift Correction		Insert Row & Avg		Calculations!		file.rep		
	X = Not Reportable						R	R	R	R	R	X	R	R	R	R	R	X	X
	Detection Limits - Screen (C)		C				100	10	10	50	50		1	0.5	1	1	0.5	0.5	0.5
	Detection Limits - Trace (B)		B				20	5	2	20	20		0.5	0.2	0.5	0.5	0.2	0.2	0.2
	Detection Limits - UltraTrace (A)		A				5	2	0.5	10	10		0.2	0.05	0.2	0.1	0.05	0.05	0.05
		Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns for Calculations to be valid													
	Units / Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested	Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45	Mn 55	Co 59	Ni 60	Cu 63	Pb 206	Pb 207	Pb 208
	Cal Blank			1.0	1							100							
	Cal Std			1.0	1		2000.00	2000.00	200.00	2000.00	2000.00	100	200.00	200.00	200.00	200.00	200.00	200.00	200.00
	Type 1 water from unit	BS 1		1.0	10		0.45	0.34	-0.06	4.97	20.45	94	0.04	0.02	0.02	-.06	0.02	.02	0.02
	Sample 1	1		99.9	10		-0.13	1.17	0.57	2.34	14.46	99	0.03	0.01	0.06	0.15	1.04	.02	1.03
	Sample 2	1		101.2	100		2.74	2.21	2.21	3.89	18.36	100	2.01	1.95	2.14	2.16	2.00	1.95	2.01
	Sample 3a			1.0	1		5450.34	2495.74	51.13	844.22	10292.98	96	4.34	0.06	0.84	9.40	0.08	0.08	0.08
	Sample 3b			1.0	1		5346.97	2423.90	49.59	830.25	10126.50	99	4.11	0.06	0.82	9.26	0.08	0.07	0.08
	Sample 3c			1.0	1		5289.07	2404.86	49.71	832.94	10024.73	97	4.15	0.07	0.86	9.81	0.07	0.08	0.08
	Avg of last 3 samples			1.0	1		5362.13	2441.50	50.14	835.80	10148.07	97	4.20	0.06	0.84	9.49	0.08	0.08	0.08
	0.5% HNO3 Blank			1.0	1		3.58	0.15	0.17	6.57	64.78	88	0.08	0.01	0.06	0.08	0.00	0.00	0.00
	Spiked Sample			1.0	1		1999.83	2026.06	202.53	2036.88	2093.66	93	201.42	200.15	203.48	199.63	187.08	187.31	187.13
	Sample 4			1.0	1		35372.18	2.13	2.23	53.74	166.76	88	0.28	0.03	1.30	1.63	0.05	0.05	0.05
	Sample 5			1.0	1		10353.27	2044.07	4.17	1962.87	9731.83	90	1060.72	0.03	1.14	5.25	0.06	0.06	0.06
	Sample 6			1.0	1		809.18	0.62	50.07	9.54	70.77	87	5.73	0.03	28.46	31.67	18.92	18.98	19.08
	1% HNO3 blank			1.0	1		4.71	0.47	0.92	6.32	63.15	92	0.11	0.02	0.07	.06	0.01	.01	0.01
	100ppm Ca			1.0	1		15.73	5.88	1.40	19.29	98927.57	91	0.46	0.15	3.62	.09	0.10	.07	0.08
	Blank as sample			1.0	1		0.43	0.33	0.52	9.59	62.63	96	0.11	0.01	0.08	.11	0.00	.00	0.00
	Std as sample			1.0	1		1999.83	2026.06	202.53	2036.88	2093.66	93	201.42	200.15	203.48	199.63	187.08	187.31	187.13

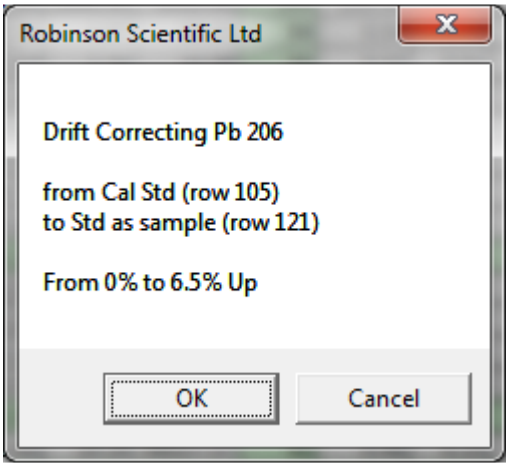






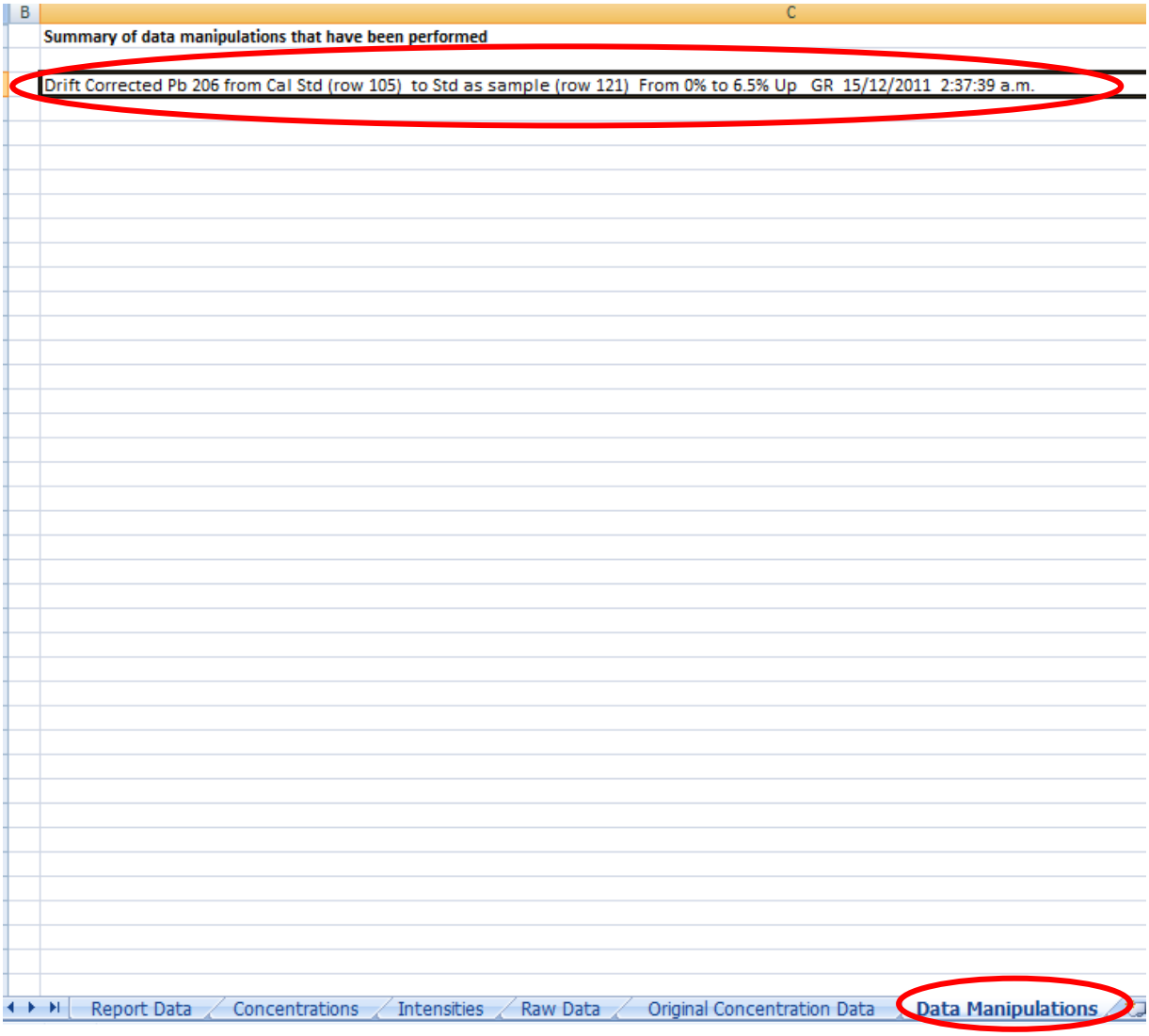






[Please see next page]

This correction has now been saved in the Data Manipulations tab:



Baseline Correction

This is the same procedure as Drift Correction above, but is designed to correct for memory effects, or an isotope washing out from a previous run, e.g. data has become negative.

Once again, Blanket or Drift correction options can be performed.

Please note: only one column can be corrected at a time. You must be on the **Concentrations** tab to perform drift or baseline corrections.

Note for Drift and Baseline Corrections: any corrections that are performed are automatically audit trailed – in other words a time and date stamped record is stored on the Data Manipulations tab of the spreadsheet.

User Defined Detection Limits

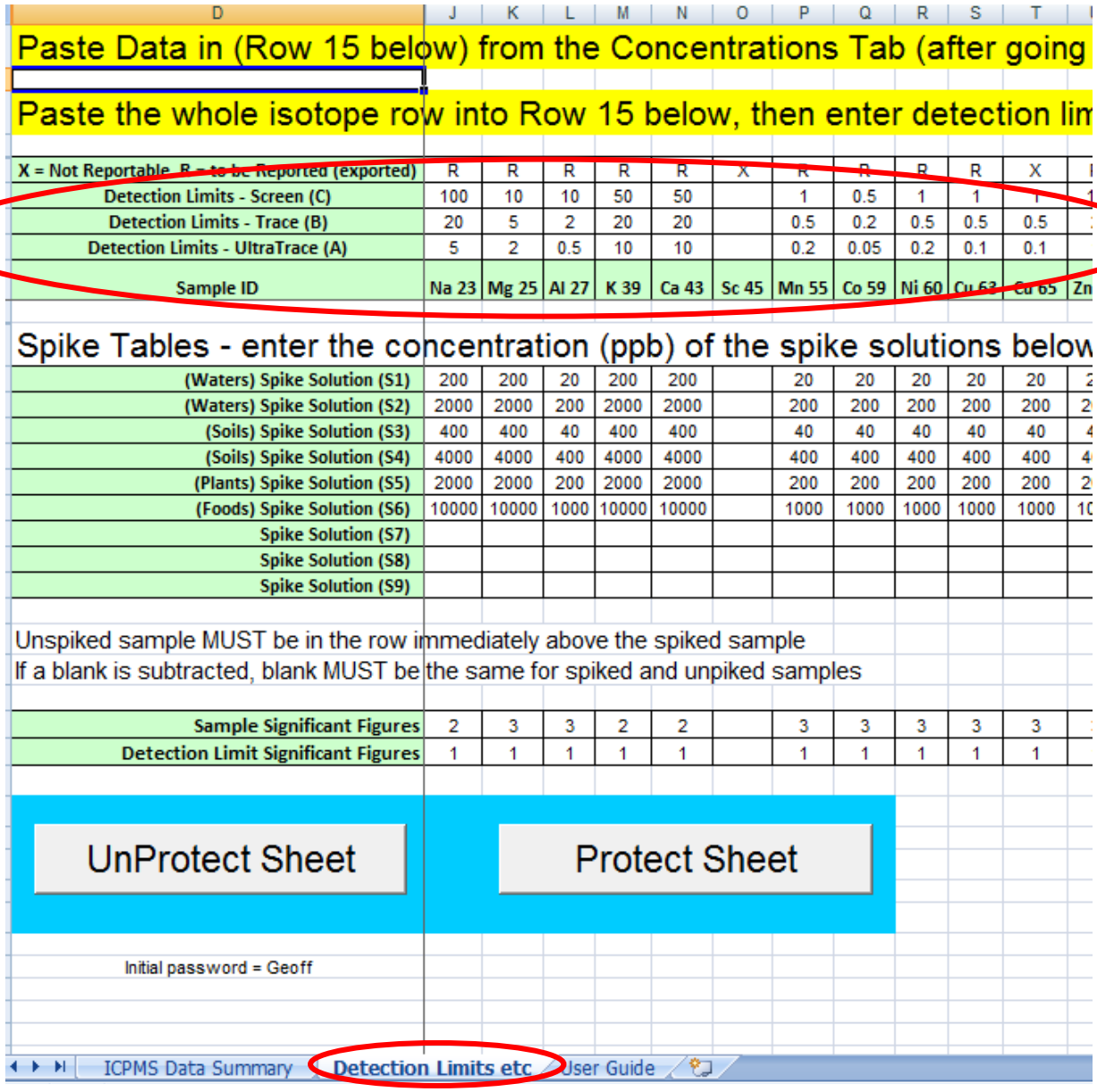
In the main Data Processing program, it is possible to define detection limits, to be compared to the data is desired.

Any results less than your chosen detection limit will be shown on the Report Data tab as <DL, see example below:

Example – setting up user defined detection limits in the main program:

[Please see next page]

Example – setting up user defined detection limits:



You can define 3 different levels of detection limits, for example screen, trace and ultratrace. (If you need more than this, you can save the main program with a different name and set up different data on other 'versions').

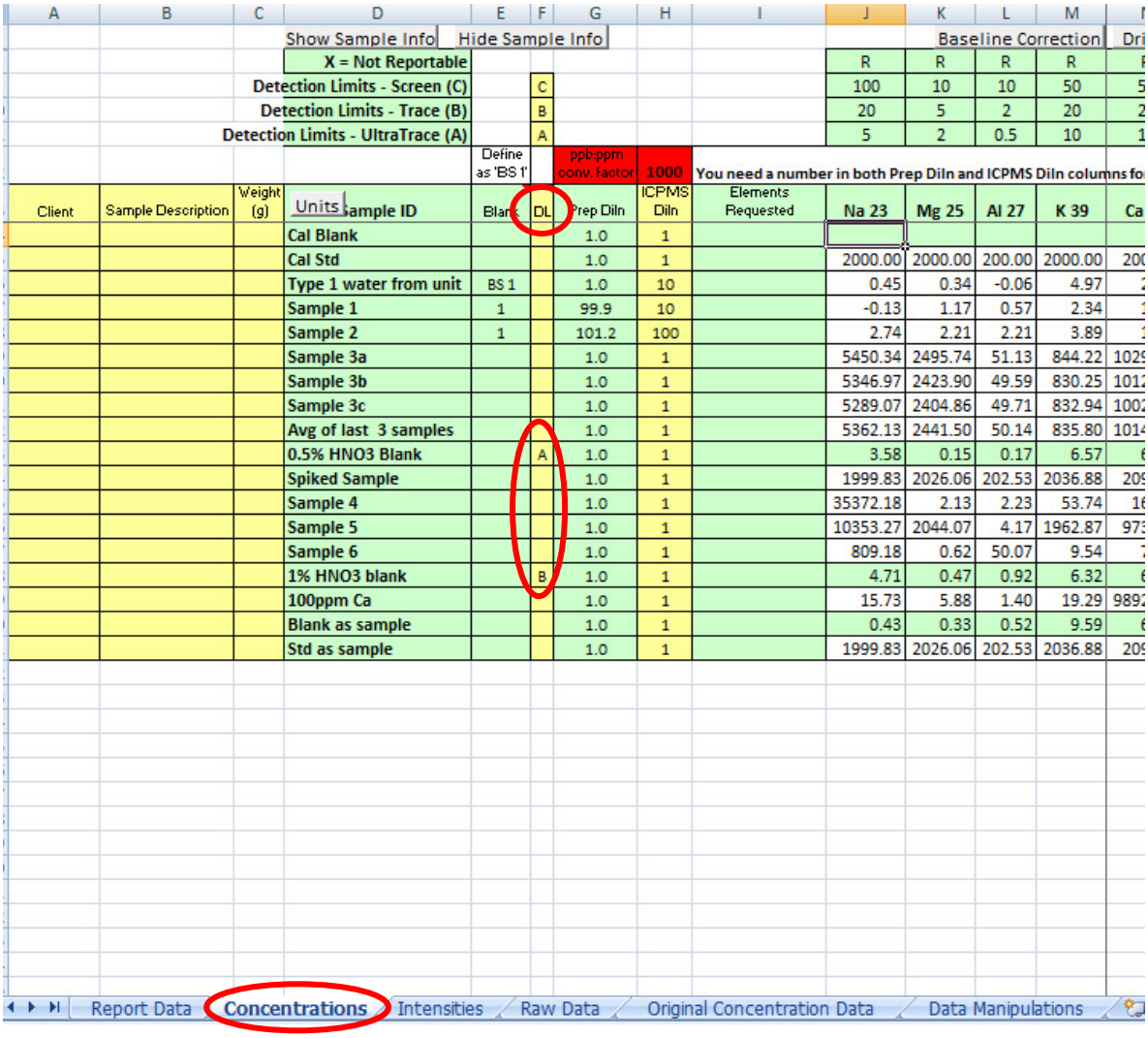
Procedure: in the main program, on the **Detection Limits etc** tab, paste (or type) the isotopes you measure (your most extensive set) into Row 15 – this data is used to match up against the data in each spreadsheet, so the names need to be what you normally use. You may have multiple names for the same isotope.

Next enter data into rows 12, 13 and 14 – this is your desired detection limit data. You may name these rows (in Column D) anything you like. These names are what will be imported into each spreadsheet when you import the data.

Once you've set up your desired detection limits, these will all be automatically imported with each set of data, when you click on the **Go To Processing** button.

To apply a detection limit to a sample (for that row) simply enter “A”, “B” or “C” in the appropriate row, as shown in the example below:

Example – applying detection limits – define appropriate detection limit in the Concentrations tab:



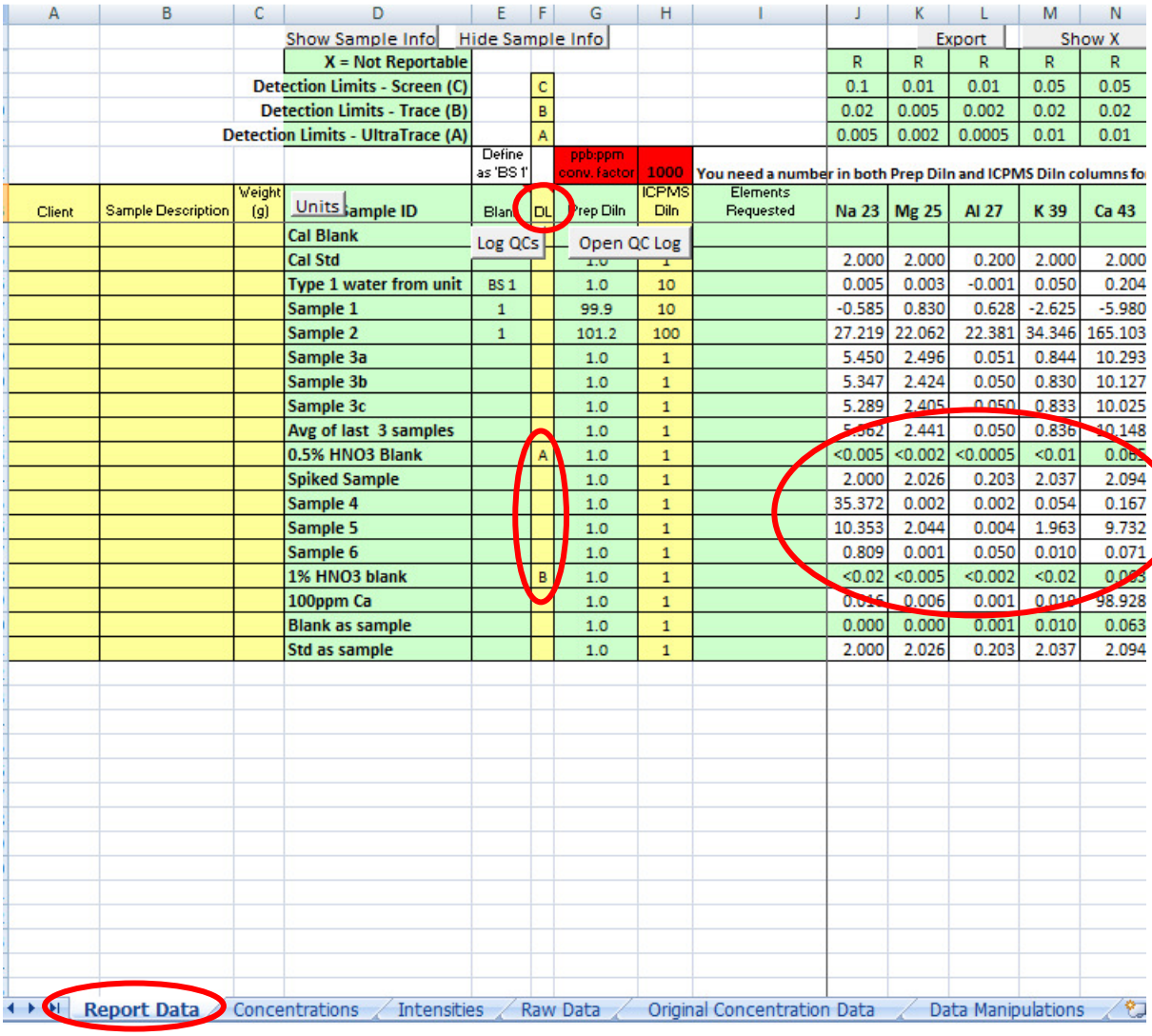
			Show Sample Info	Hide Sample Info								Baseline Correction			Dri
			X = Not Reportable							R	R	R	R	R	
			Detection Limits - Screen (C)		C					100	10	10	50	5	
			Detection Limits - Trace (B)		B					20	5	2	20	2	
			Detection Limits - UltraTrace (A)		A					5	2	0.5	10	1	
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns fo							
Client	Sample Description	Weight (g)	Units Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested		Na 23	Mg 25	Al 27	K 39	Ca	
			Cal Blank			1.0	1								
			Cal Std			1.0	1			2000.00	2000.00	200.00	2000.00	200	
			Type 1 water from unit	BS 1		1.0	10			0.45	0.34	-0.06	4.97		
			Sample 1	1		99.9	10			-0.13	1.17	0.57	2.34		
			Sample 2	1		101.2	100			2.74	2.21	2.21	3.89		
			Sample 3a			1.0	1			5450.34	2495.74	51.13	844.22	1029	
			Sample 3b			1.0	1			5346.97	2423.90	49.59	830.25	1012	
			Sample 3c			1.0	1			5289.07	2404.86	49.71	832.94	1002	
			Avg of last 3 samples			1.0	1			5362.13	2441.50	50.14	835.80	1014	
			0.5% HNO3 Blank		A	1.0	1			3.58	0.15	0.17	6.57	6	
			Spiked Sample			1.0	1			1999.83	2026.06	202.53	2036.88	209	
			Sample 4			1.0	1			35372.18	2.13	2.23	53.74	16	
			Sample 5			1.0	1			10353.27	2044.07	4.17	1962.87	973	
			Sample 6			1.0	1			809.18	0.62	50.07	9.54	7	
			1% HNO3 blank		B	1.0	1			4.71	0.47	0.92	6.32	6	
			100ppm Ca			1.0	1			15.73	5.88	1.40	19.29	9892	
			Blank as sample			1.0	1			0.43	0.33	0.52	9.59	6	
			Std as sample			1.0	1			1999.83	2026.06	202.53	2036.88	209	

Report Data | Concentrations | Intensities | Raw Data | Original Concentration Data | Data Manipulations

When you click on the **Calculations!** button the concentration data will be compared to the corresponding detection limit, and shown as less than that detection limit (if it is) on the Report Data tab. See example below:

[Please see next page]

Example – applying detection limits – samples shown compared to the detection limit in the Report Data tab:



			Show Sample Info	Hide Sample Info							Export		Show X	
			X = Not Reportable						R	R	R	R	R	
			Detection Limits - Screen (C)		C				0.1	0.01	0.01	0.05	0.05	
			Detection Limits - Trace (B)		B				0.02	0.005	0.002	0.02	0.02	
			Detection Limits - UltraTrace (A)		A				0.005	0.002	0.0005	0.01	0.01	
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns fo						
Client	Sample Description	Weight (g)	Units Sample ID	Blan	DL	Prep Diln	ICPMS Diln	Elements Requested	Na 23	Mg 25	Al 27	K 39	Ca 43	
			Cal Blank	Log QCs		Open QC Log								
			Cal Std						2.000	2.000	0.200	2.000	2.000	
			Type 1 water from unit	BS 1		1.0	10		0.005	0.003	-0.001	0.050	0.204	
			Sample 1	1		99.9	10		-0.585	0.830	0.628	-2.625	-5.980	
			Sample 2	1		101.2	100		27.219	22.062	22.381	34.346	165.103	
			Sample 3a			1.0	1		5.450	2.496	0.051	0.844	10.293	
			Sample 3b			1.0	1		5.347	2.424	0.050	0.830	10.127	
			Sample 3c			1.0	1		5.289	2.405	0.050	0.833	10.025	
			Avg of last 3 samples			1.0	1		5.362	2.441	0.050	0.836	10.148	
			0.5% HNO3 Blank		A	1.0	1		<0.005	<0.002	<0.0005	<0.01	0.065	
			Spiked Sample			1.0	1		2.000	2.026	0.203	2.037	2.094	
			Sample 4			1.0	1		35.372	0.002	0.002	0.054	0.167	
			Sample 5			1.0	1		10.353	2.044	0.004	1.963	9.732	
			Sample 6			1.0	1		0.809	0.001	0.050	0.010	0.071	
			1% HNO3 blank		B	1.0	1		<0.02	<0.005	<0.002	<0.02	0.093	
			100ppm Ca			1.0	1		0.016	0.006	0.001	0.019	98.928	
			Blank as sample			1.0	1		0.000	0.000	0.001	0.010	0.063	
			Std as sample			1.0	1		2.000	2.026	0.203	2.037	2.094	

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[Please see next page]

User Defined Significant Figures

As for the Detection Limit data, this is set up on the Detection Limits etc tab of the main program. It is imported and applied to each set of data when you click on the **Go To Processing** button.

Data with your chosen significant figures applied is shown on the **Report Data** tab of the spreadsheet, but **ONLY** for samples with a DL (detection limit) defined.

Example – user defined significant figures:

Paste Data in (Row 15 below) from the Concentrations Tab (after going

Paste the whole isotope row into Row 15 below, then enter detection lim

X = Not Reportable, R = to be Reported (exported)	R	R	R	R	R	X	R	R	R	R	X
Detection Limits - Screen (C)	100	10	10	50	50		1	0.5	1	1	1
Detection Limits - Trace (B)	20	5	2	20	20		0.5	0.2	0.5	0.5	0.5
Detection Limits - UltraTrace (A)	5	2	0.5	10	10		0.2	0.05	0.2	0.1	0.1
Sample ID	Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45	Mn 55	Co 59	Ni 60	Cu 63	Cu 65

Spike Tables - enter the concentration (ppb) of the spike solutions below

(Waters) Spike Solution (S1)	200	200	20	200	200		20	20	20	20	20
(Waters) Spike Solution (S2)	2000	2000	200	2000	2000		200	200	200	200	200
(Soils) Spike Solution (S3)	400	400	40	400	400		40	40	40	40	40
(Soils) Spike Solution (S4)	4000	4000	400	4000	4000		400	400	400	400	400
(Plants) Spike Solution (S5)	2000	2000	200	2000	2000		200	200	200	200	200
(Foods) Spike Solution (S6)	10000	10000	1000	10000	10000		1000	1000	1000	1000	1000
Spike Solution (S7)											
Spike Solution (S8)											
Spike Solution (S9)											

Unspiked sample MUST be in the row immediately above the spiked sample
If a blank is subtracted, blank MUST be the same for spiked and unpiked samples

Sample Significant Figures	2	3	3	2	2		3	3	3	3	3
Detection Limit Significant Figures	1	1	1	1	1		1	1	1	1	1

UnProtect Sheet Protect Sheet

Initial password = Geoff

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[Please see next page]

Automatic Spike Recovery Calculations

Spike Recoveries can be automatically calculated for samples.

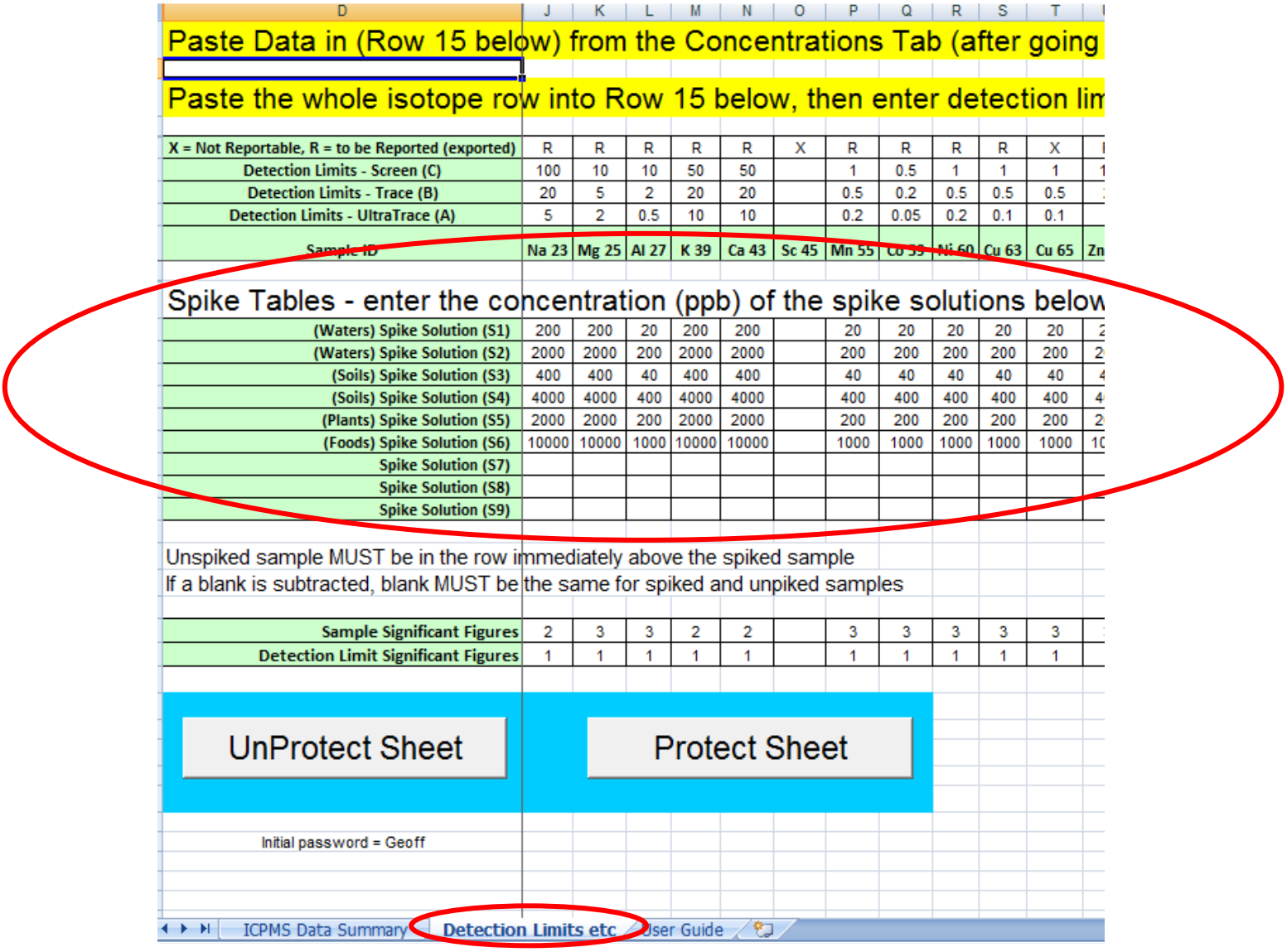
Once again, the data for this is set up on the Detection Limits etc tab of the main program. You may have up to 9 different spiking levels.

Please note: the unspiked sample MUST be in the row immediately above the spiked sample (this is an assumption made in the calculations).

Please note: if a blank is subtracted from the spiked sample, the blank MUST be the same for the spiked and unspiked samples (this would be good practice anyway).

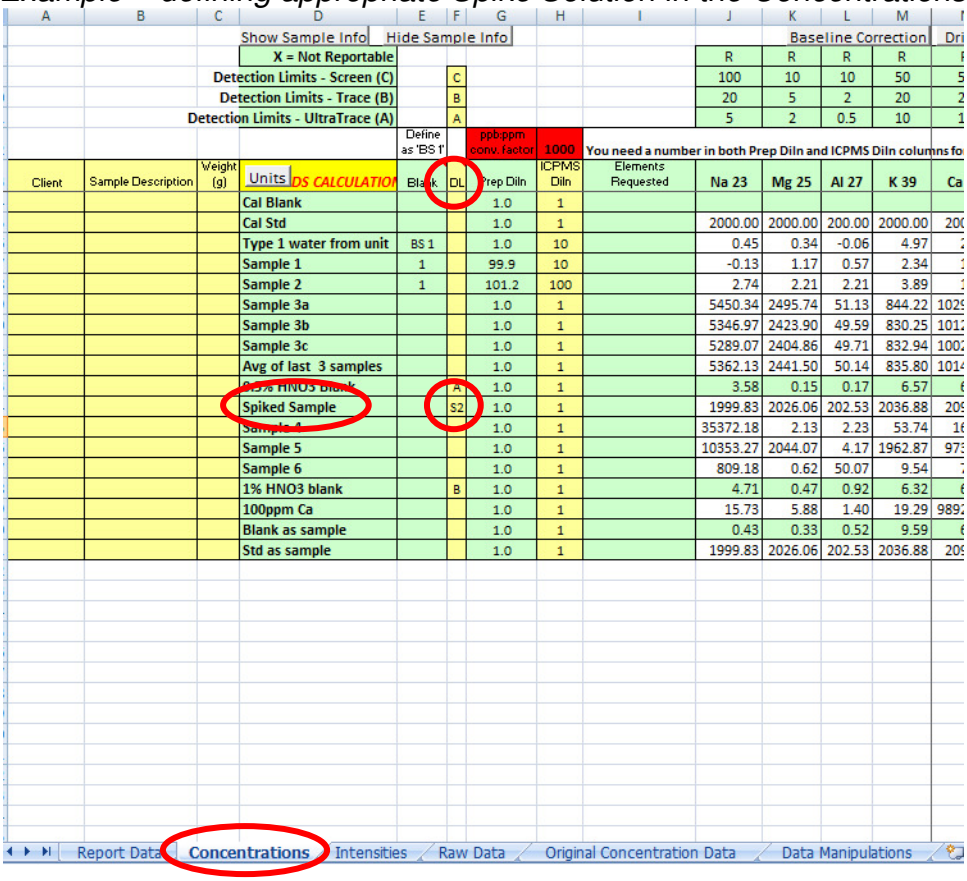
Procedure: simply enter the spike number for the spike you wish to use (S1 to S9) into the DL column (Column F) on the **Concentrations** tab, in the format e.g. **S1** for spike solution 1. When you click on the **Calculations!** button the spike recovery will be shown on the **Report Data** tab. Please see example below:

Example – setting up spike recovery tables:



D	J	K	L	M	N	O	P	Q	R	S	T
Paste Data in (Row 15 below) from the Concentrations Tab (after going											
Paste the whole isotope row into Row 15 below, then enter detection lim											
X = Not Reportable, R = to be Reported (exported)	R	R	R	R	R	X	R	R	R	R	X
Detection Limits - Screen (C)	100	10	10	50	50		1	0.5	1	1	1
Detection Limits - Trace (B)	20	5	2	20	20		0.5	0.2	0.5	0.5	0.5
Detection Limits - UltraTrace (A)	5	2	0.5	10	10		0.2	0.05	0.2	0.1	0.1
Sample ID	Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45	Mn 55	Co 59	Ni 60	Cu 63	Cu 65
Spike Tables - enter the concentration (ppb) of the spike solutions below											
(Waters) Spike Solution (S1)	200	200	20	200	200		20	20	20	20	20
(Waters) Spike Solution (S2)	2000	2000	200	2000	2000		200	200	200	200	200
(Soils) Spike Solution (S3)	400	400	40	400	400		40	40	40	40	40
(Soils) Spike Solution (S4)	4000	4000	400	4000	4000		400	400	400	400	400
(Plants) Spike Solution (S5)	2000	2000	200	2000	2000		200	200	200	200	200
(Foods) Spike Solution (S6)	10000	10000	1000	10000	10000		1000	1000	1000	1000	1000
Spike Solution (S7)											
Spike Solution (S8)											
Spike Solution (S9)											
Unspiked sample MUST be in the row immediately above the spiked sample											
If a blank is subtracted, blank MUST be the same for spiked and unpiked samples											
Sample Significant Figures	2	3	3	2	2		3	3	3	3	3
Detection Limit Significant Figures	1	1	1	1	1		1	1	1	1	1

Example – defining appropriate Spike Solution in the Concentrations tab:



			Show Sample Info	Hide Sample Info							Baseline Correction				
			X = Not Reportable							R	R	R	R	R	
			Detection Limits - Screen (C)		C					100	10	10	50	5	
			Detection Limits - Trace (B)		B					20	5	2	20	2	
			Detection Limits - UltraTrace (A)		A					5	2	0.5	10	1	
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns fo							
Client	Sample Description	Weight (g)	Units DS CALCULATIO	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested		Na 23	Mg 25	Al 27	K 39	Ca	
			Cal Blank			1.0	1								
			Cal Std			1.0	1			2000.00	2000.00	200.00	2000.00	200	
			Type 1 water from unit	BS 1		1.0	10			0.45	0.34	-0.06	4.97	2	
			Sample 1	1		99.9	10			-0.13	1.17	0.57	2.34	1	
			Sample 2	1		101.2	100			2.74	2.21	2.21	3.89	1	
			Sample 3a			1.0	1			5450.34	2495.74	51.13	844.22	1025	
			Sample 3b			1.0	1			5346.97	2423.90	49.59	830.25	1012	
			Sample 3c			1.0	1			5289.07	2404.86	49.71	832.94	1002	
			Avg of last 3 samples			1.0	1			5362.13	2441.50	50.14	835.80	1014	
			0.5% HNO3 Blank		A	1.0	1			3.58	0.15	0.17	6.57	6	
			Spiked Sample		S2	1.0	1			1999.83	2026.06	202.53	2036.88	205	
			Sample 4			1.0	1			35372.18	2.13	2.23	53.74	16	
			Sample 5			1.0	1			10353.27	2044.07	4.17	1962.87	973	
			Sample 6			1.0	1			809.18	0.62	50.07	9.54	7	
			1% HNO3 blank		B	1.0	1			4.71	0.47	0.92	6.32	6	
			100ppm Ca			1.0	1			15.73	5.88	1.40	19.29	9892	
			Blank as sample			1.0	1			0.43	0.33	0.52	9.59	6	
			Std as sample			1.0	1			1999.83	2026.06	202.53	2036.88	205	

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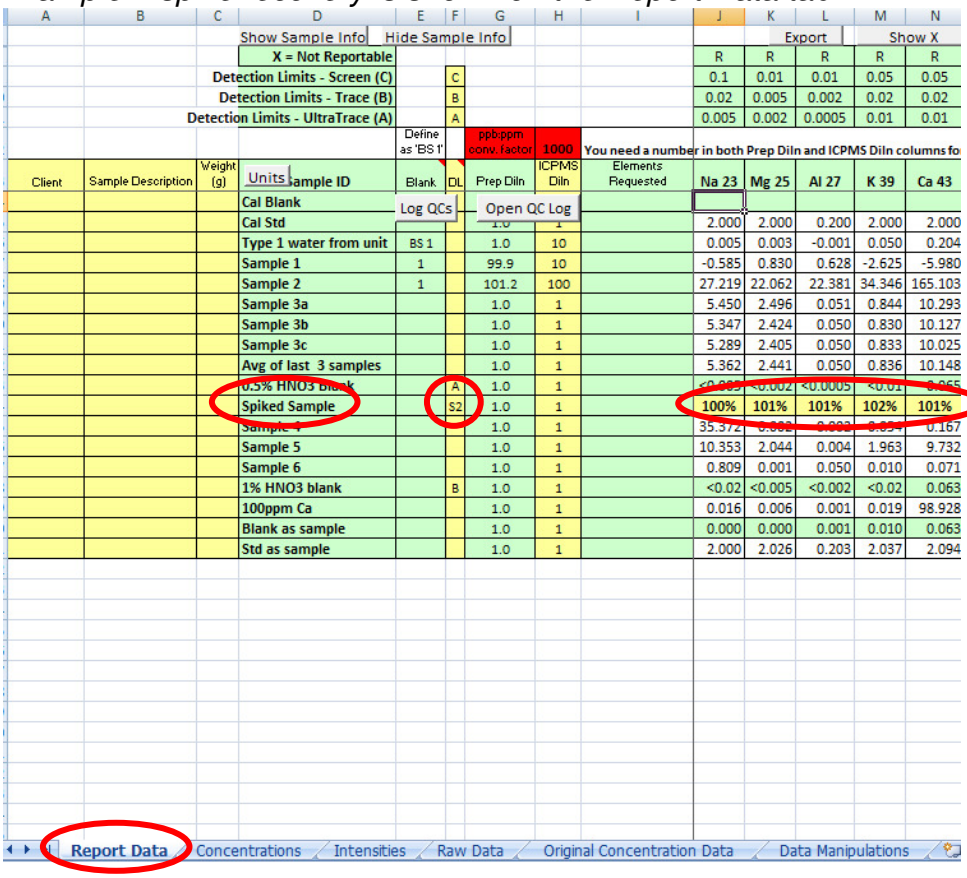
Example – spike recovery is shown on the Report Data tab:



			Show Sample Info	Hide Sample Info							Export		Show X		
			X = Not Reportable							R	R	R	R	R	
			Detection Limits - Screen (C)		C					0.1	0.01	0.01	0.05	0.05	
			Detection Limits - Trace (B)		B					0.02	0.005	0.002	0.02	0.02	
			Detection Limits - UltraTrace (A)		A					0.005	0.002	0.0005	0.01	0.01	
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns fo							
Client	Sample Description	Weight (g)	Units ample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested		Na 23	Mg 25	Al 27	K 39	Ca 43	
			Cal Blank	Log QCs		Open QC Log									
			Cal Std			1.0	1			2.000	2.000	0.200	2.000	2.000	
			Type 1 water from unit	BS 1		1.0	10			0.005	0.003	-0.001	0.050	0.204	
			Sample 1	1		99.9	10			-0.585	0.830	0.628	-2.625	-5.980	
			Sample 2	1		101.2	100			27.219	22.062	22.381	34.346	165.103	
			Sample 3a			1.0	1			5.450	2.496	0.051	0.844	10.293	
			Sample 3b			1.0	1			5.347	2.424	0.050	0.830	10.127	
			Sample 3c			1.0	1			5.289	2.405	0.050	0.833	10.025	
			Avg of last 3 samples			1.0	1			5.362	2.441	0.050	0.836	10.148	
			0.5% HNO3 Blank		A	1.0	1			<0.005	<0.002	<0.0005	<0.01	0.055	
			Spiked Sample		S2	1.0	1			100%	101%	101%	102%	101%	
			Sample 4			1.0	1			35.372	0.008	0.003	0.054	0.167	
			Sample 5			1.0	1			10.353	2.044	0.004	1.963	9.732	
			Sample 6			1.0	1			0.809	0.001	0.050	0.010	0.071	
			1% HNO3 blank		B	1.0	1			<0.02	<0.005	<0.002	<0.02	0.063	
			100ppm Ca			1.0	1			0.016	0.006	0.001	0.019	98.928	
			Blank as sample			1.0	1			0.000	0.000	0.001	0.010	0.063	
			Std as sample			1.0	1			2.000	2.026	0.203	2.037	2.094	

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Show / Hide isotopes of interest

On the **Report Data** tab of the spreadsheet you can quickly show or hide isotopes of interest, simply by clicking on the **Show X Columns** button or the **Hide X** button. All isotopes are initially shown by default.

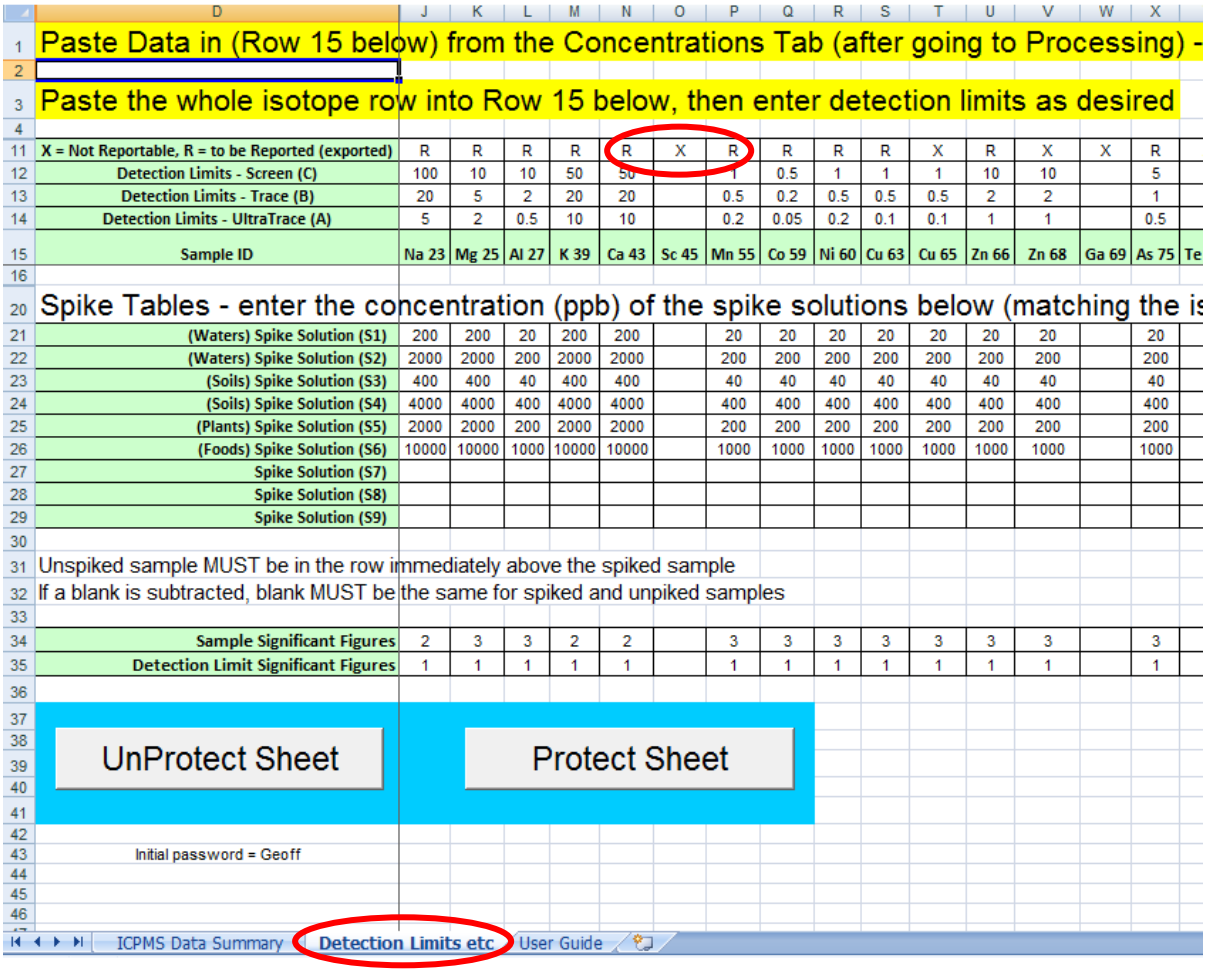
Terminology: X is defined as "not reportable" but this really just means "not of interest".

Procedure: isotopes are defined as not of interest (enter "X") or of interest (enter "R") in row 11 of the main program, on the Detection Limits etc tab.

*Setting up Isotopes of Interest – first select the **Detection Limits etc** tab as shown:*

[Please see next page]

Next enter "R" or "X" – "R" for Reportable (of interest) or "X" for not of interest, e.g. an internal standard, or isotope only being monitored but not reported etc:



	D	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X
1	Paste Data in (Row 15 below) from the Concentrations Tab (after going to Processing) -															
2																
3	Paste the whole isotope row into Row 15 below, then enter detection limits as desired															
4																
11	X = Not Reportable, R = to be Reported (exported)	R	R	R	R	R	X	R	R	R	R	X	R	X	X	R
12	Detection Limits - Screen (C)	100	10	10	50	50		1	0.5	1	1	1	10	10		5
13	Detection Limits - Trace (B)	20	5	2	20	20		0.5	0.2	0.5	0.5	0.5	2	2		1
14	Detection Limits - UltraTrace (A)	5	2	0.5	10	10		0.2	0.05	0.2	0.1	0.1	1	1		0.5
15	Sample ID	Na 23	Mg 25	Al 27	K 39	Ca 43	Sc 45	Mn 55	Co 59	Ni 60	Cu 63	Cu 65	Zn 66	Zn 68	Ga 69	As 75
16																
20	Spike Tables - enter the concentration (ppb) of the spike solutions below (matching the is															
21	(Waters) Spike Solution (S1)	200	200	20	200	200		20	20	20	20	20	20	20		20
22	(Waters) Spike Solution (S2)	2000	2000	200	2000	2000		200	200	200	200	200	200	200		200
23	(Soils) Spike Solution (S3)	400	400	40	400	400		40	40	40	40	40	40	40		40
24	(Soils) Spike Solution (S4)	4000	4000	400	4000	4000		400	400	400	400	400	400	400		400
25	(Plants) Spike Solution (S5)	2000	2000	200	2000	2000		200	200	200	200	200	200	200		200
26	(Foods) Spike Solution (S6)	10000	10000	1000	10000	10000		1000	1000	1000	1000	1000	1000	1000		1000
27	Spike Solution (S7)															
28	Spike Solution (S8)															
29	Spike Solution (S9)															
30																
31	Unspiked sample MUST be in the row immediately above the spiked sample															
32	If a blank is subtracted, blank MUST be the same for spiked and unpiked samples															
33																
34	Sample Significant Figures	2	3	3	2	2		3	3	3	3	3	3	3		3
35	Detection Limit Significant Figures	1	1	1	1	1		1	1	1	1	1	1	1		1
36																
37	UnProtect Sheet							Protect Sheet								
43	Initial password = Geoff															

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Automatic QC Logging

You may define a QC log name and location, on the front page of the main program.

Once you have a QC log defined, simply enter "**Q**" (without the quotes) in the DL (detection limit) column on the **Concentrations** tab (see example below). Then from the **Report Data** tab, you can open your QC log if you wish by clicking on the **Open QC Log** button, or automatically log all QC's (defined by having entered "Q" in that column), simply by clicking on the **Log QCs** button. This automatically opens your QC log, and **if it finds a tab with the same name as that QC**, your QC will automatically be added to the bottom of that tab.

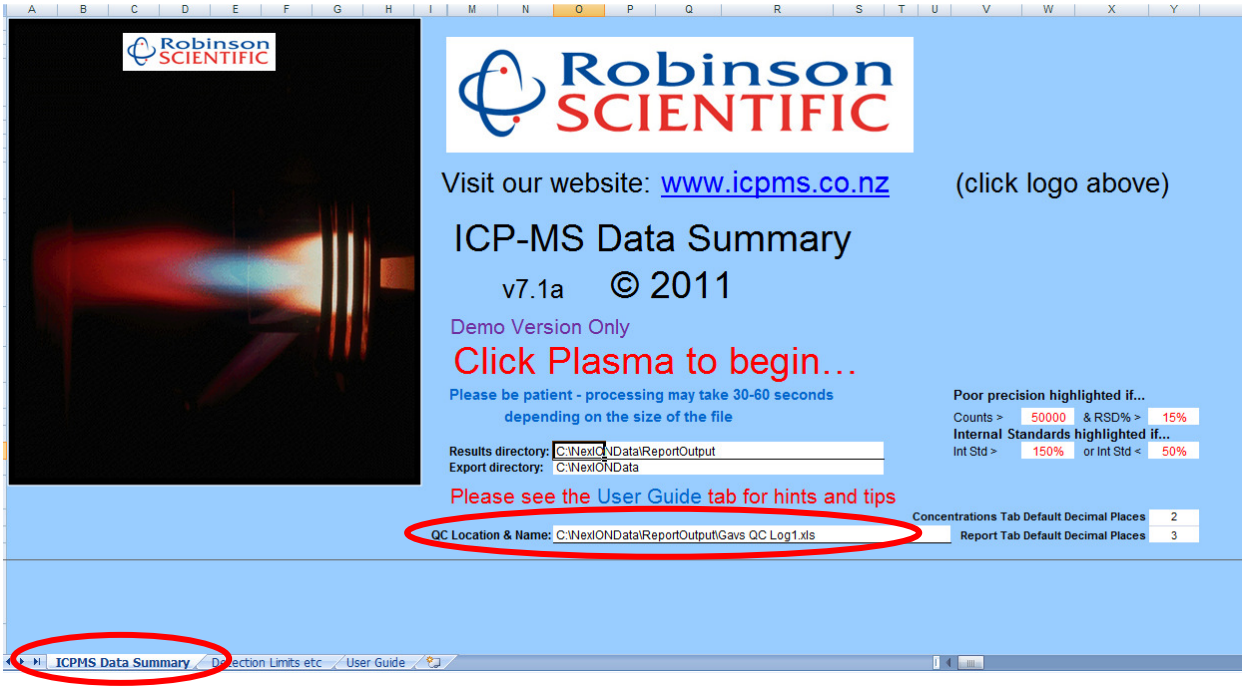
Setting up a QC log: you can start with the Example QC Log available from Robinson Scientific, or create your own. Simply ensure that you have copied the isotope row from your data spreadsheet, into **row 103** of a spreadsheet, then data will be added automatically from **row 104** onwards. Above row 103, things can be set up as you wish, rows hidden etc. Ensure you copy this sheet so you have a tab for each QC you wish to log, named the same as what you will call your QC in the spreadsheet.

Automatic QC Logging (continued)

Please Note: when QC's are automatically logged, the whole row of data is added to the appropriate tab of the QC Log. There is no check against the isotope info, so please ensure the isotopes set up in your QC log accurately match the isotopes in your analysis run (the data processing spreadsheet, Report Data tab). On the QC log you can easily hide columns, as long as they are present in the background to ensure the isotopes match up correctly.

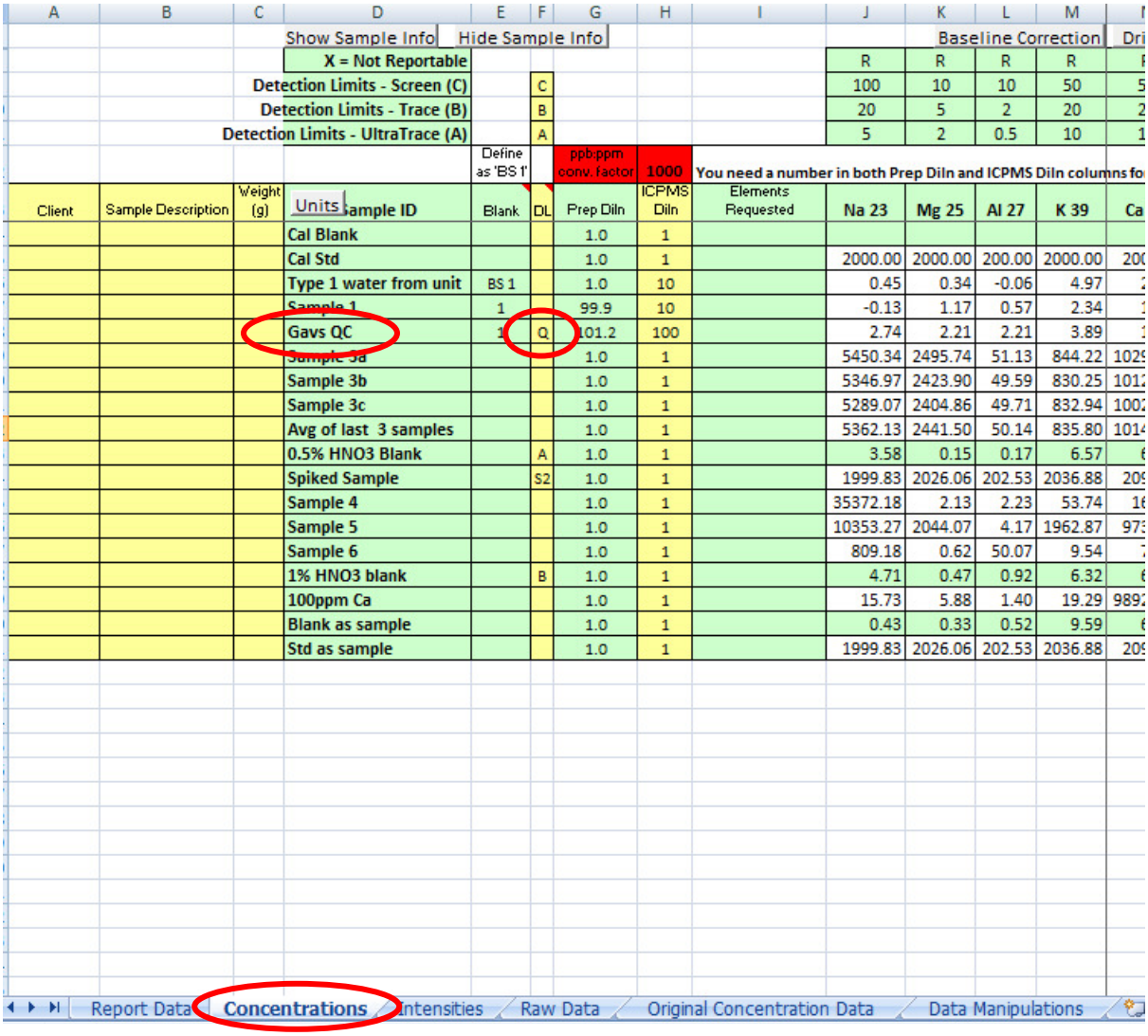
Please see example below.

Example – defining QC name and file location:



[Please see next page]

Example – defining QC to be logged (in the Concentrations tab):



			Show Sample Info	Hide Sample Info							Baseline Correction			Dri
			X = Not Reportable						R	R	R	R		
			Detection Limits - Screen (C)		C				100	10	10	50		5
			Detection Limits - Trace (B)		B				20	5	2	20		2
			Detection Limits - UltraTrace (A)		A				5	2	0.5	10		1
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns fo						
Client	Sample Description	Weight (g)	Units Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested	Na 23	Mg 25	Al 27	K 39	Ca	
			Cal Blank			1.0	1							
			Cal Std			1.0	1		2000.00	2000.00	200.00	2000.00	200	
			Type 1 water from unit	BS 1		1.0	10		0.45	0.34	-0.06	4.97		
			Sample 1	1		99.9	10		-0.13	1.17	0.57	2.34		
			Gavs QC	1	Q	101.2	100		2.74	2.21	2.21	3.89		
			Sample 3a			1.0	1		5450.34	2495.74	51.13	844.22	1029	
			Sample 3b			1.0	1		5346.97	2423.90	49.59	830.25	1012	
			Sample 3c			1.0	1		5289.07	2404.86	49.71	832.94	1002	
			Avg of last 3 samples			1.0	1		5362.13	2441.50	50.14	835.80	1014	
			0.5% HNO3 Blank		A	1.0	1		3.58	0.15	0.17	6.57	6	
			Spiked Sample		S2	1.0	1		1999.83	2026.06	202.53	2036.88	209	
			Sample 4			1.0	1		35372.18	2.13	2.23	53.74	16	
			Sample 5			1.0	1		10353.27	2044.07	4.17	1962.87	973	
			Sample 6			1.0	1		809.18	0.62	50.07	9.54	7	
			1% HNO3 blank		B	1.0	1		4.71	0.47	0.92	6.32	6	
			100ppm Ca			1.0	1		15.73	5.88	1.40	19.29	989	
			Blank as sample			1.0	1		0.43	0.33	0.52	9.59	6	
			Std as sample			1.0	1		1999.83	2026.06	202.53	2036.88	209	

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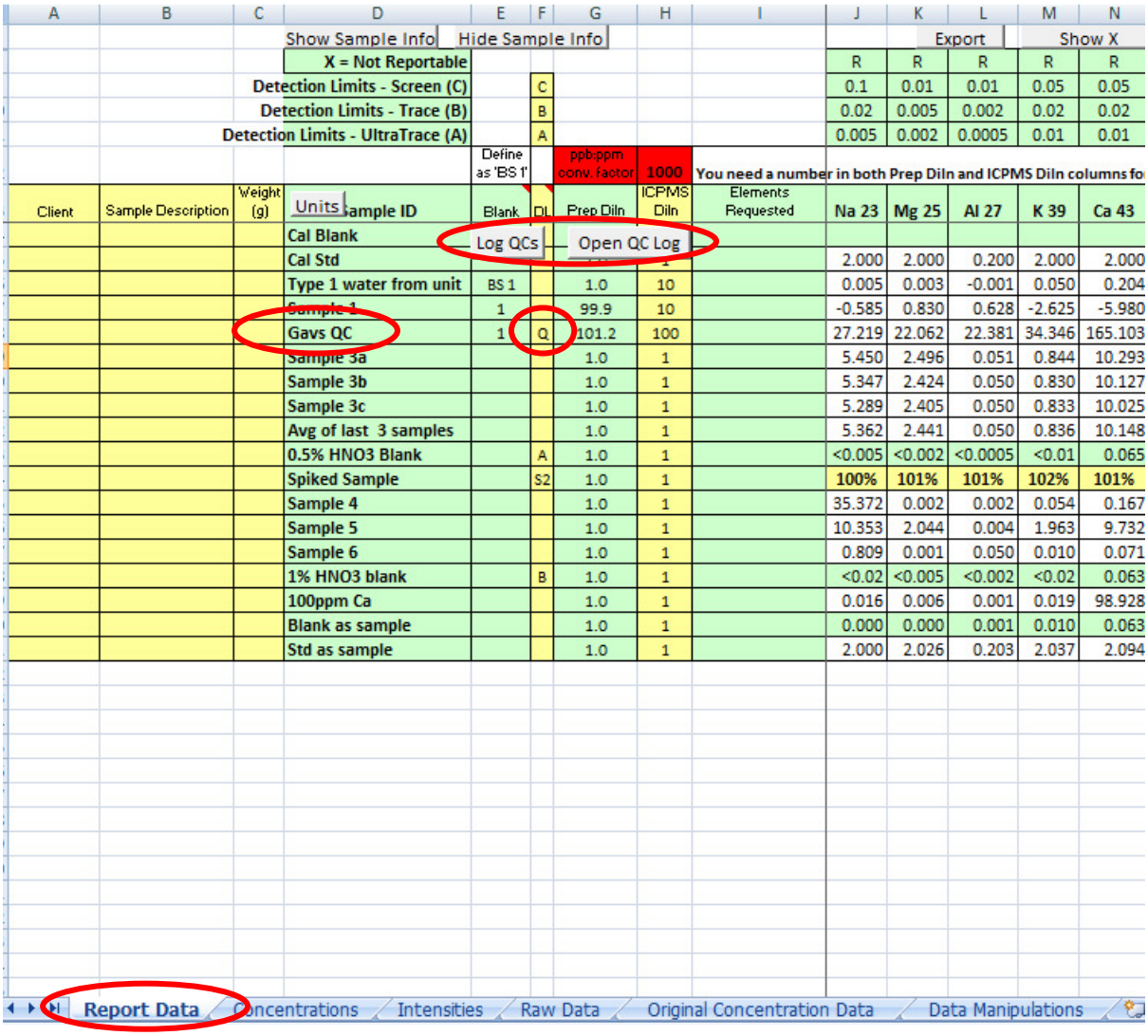
[Please see next page]

Example – ready to Log the QC (all QCs) (on the Report Data tab) by clicking the Log QCs button:



			Show Sample Info / Hide Sample Info								Export		Show X	
			X = Not Reportable						R	R	R	R	R	
			Detection Limits - Screen (C)		C				0.1	0.01	0.01	0.05	0.05	
			Detection Limits - Trace (B)		B				0.02	0.005	0.002	0.02	0.02	
			Detection Limits - UltraTrace (A)		A				0.005	0.002	0.0005	0.01	0.01	
				Define as 'BS 1'		ppb:ppm conv. factor	1000	You need a number in both Prep Diln and ICPMS Diln columns fo						
Client	Sample Description	Weight (g)	Units / Sample ID	Blank	DL	Prep Diln	ICPMS Diln	Elements Requested	Na 23	Mg 25	Al 27	K 39	Ca 43	
			Cal Blank	Log QCs		Open QC Log								
			Cal Std						2.000	2.000	0.200	2.000	2.000	
			Type 1 water from unit	BS 1		1.0	10		0.005	0.003	-0.001	0.050	0.204	
			Sample 1	1		99.9	10		-0.585	0.830	0.628	-2.625	-5.980	
			Gavs QC	1	Q	101.2	100		27.219	22.062	22.381	34.346	165.103	
			Sample 3a			1.0	1		5.450	2.496	0.051	0.844	10.293	
			Sample 3b			1.0	1		5.347	2.424	0.050	0.830	10.127	
			Sample 3c			1.0	1		5.289	2.405	0.050	0.833	10.025	
			Avg of last 3 samples			1.0	1		5.362	2.441	0.050	0.836	10.148	
			0.5% HNO3 Blank		A	1.0	1		<0.005	<0.002	<0.0005	<0.01	0.065	
			Spiked Sample		S2	1.0	1		100%	101%	101%	102%	101%	
			Sample 4			1.0	1		35.372	0.002	0.002	0.054	0.167	
			Sample 5			1.0	1		10.353	2.044	0.004	1.963	9.732	
			Sample 6			1.0	1		0.809	0.001	0.050	0.010	0.071	
			1% HNO3 blank		B	1.0	1		<0.02	<0.005	<0.002	<0.02	0.063	
			100ppm Ca			1.0	1		0.016	0.006	0.001	0.019	98.928	
			Blank as sample			1.0	1		0.000	0.000	0.001	0.010	0.063	
			Std as sample			1.0	1		2.000	2.026	0.203	2.037	2.094	

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Example – QC that has just been automatically added to QC Log:

A	B	C	D	J	K	L	M	N
Notes: (note columns E-I are hidden)			Running (Calculated) Mean	27.24	22.08	22.40	34.37	165.13
Grey = < Detection Limit			Running (Calculated) Upper Confidence Limit	27.50	22.34	22.66	34.63	165.38
Blue & Bold = outside user defined confidence limits			Running (Calculated) Lower Confidence Limit	27.24	22.08	22.40	34.37	165.13
Red & Bold = outside CRM / SRM confidence limits			User Defined QC Mean Value	27.00	22.00	22.00	34.00	165.00
			User Defined Upper Confidence Limit	30.00	25.00	25.00	40.00	180.00
			User Defined Lower Confidence Limit	25.00	19.00	19.00	27.00	155.00
			CRM / SRM Mean Value			22.5		
			CRM / SRM Upper Confidence Limit			23.5		
Update Calculations			CRM / SRM Lower Confidence Limit			21.5		
			Detection Limit	5	2	0.5	10	10
Client	Sample Description	Weight (g)	Sample ID	Na 23	Mg 25	Al 27	K 39	Ca 43
			Gavs QC	27.219	22.062	22.381	34.346	165.103
			Gavs QC	27.339	22.182	22.501	34.466	165.223
			Gavs QC	27.069	21.912	22.231	34.196	164.953
			Gavs QC	27.339	22.182	22.501	34.466	165.223

Gavs QC

[Please see next page]

OPTIONAL one button LIMS export

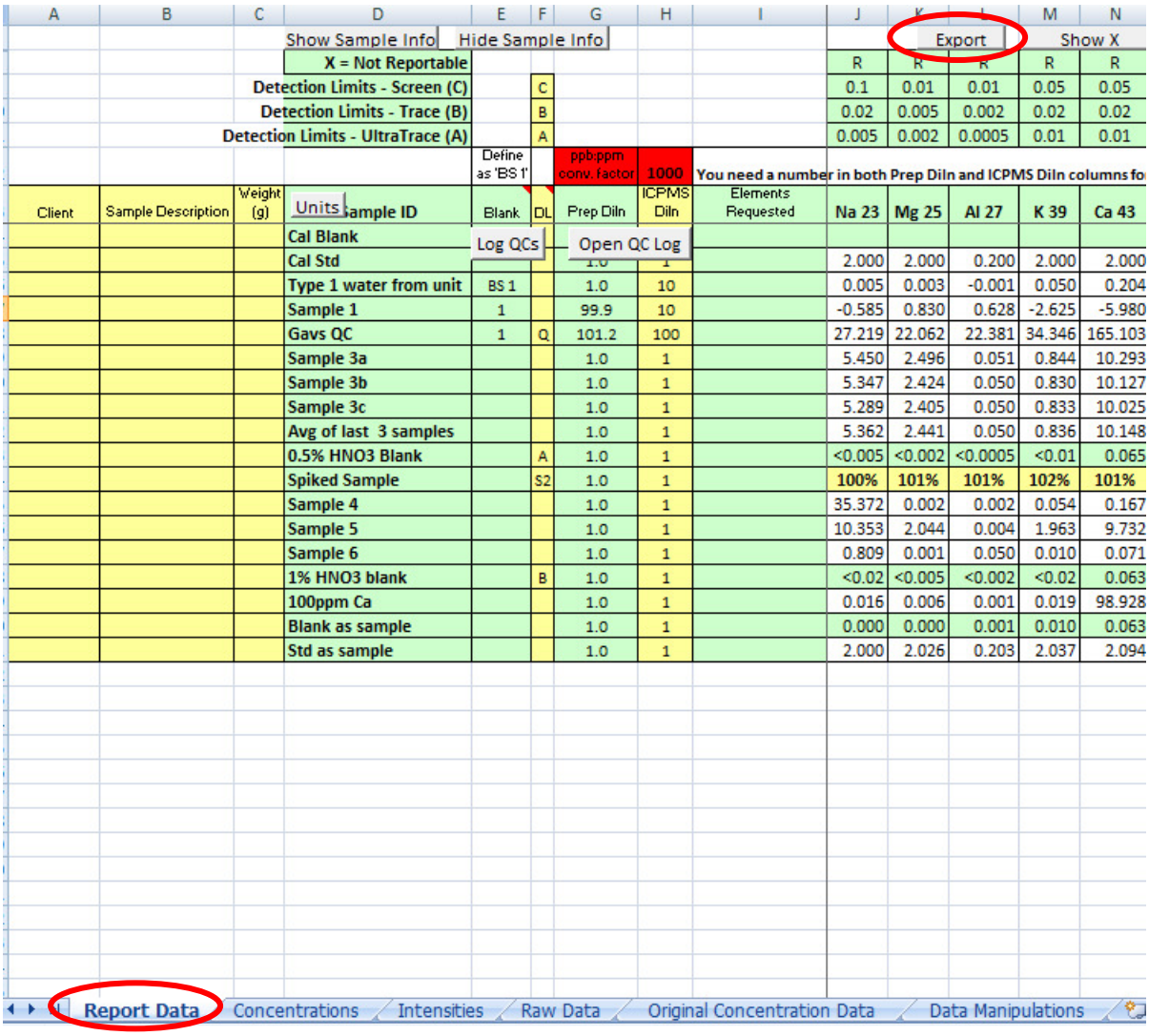
It is possible to set up the data processing program to automatically export a file to your LIMS system once you have seen and processed the data.

This is available as an option, at extra cost, as most LIMS systems have different configurations and requirements, hence there is a need for us to program this specifically to your requirements.

Please contact us to discuss this. Typical cost is $1950 for a custom configuration.

Please see example below (a file exported ready for LabWare in this case):

Example – LIMS export file button:



Example – typical LIMS export file (generated by clicking the Export button):

	A	B	C	D	E	F
1	Sample.Text_ID	Test.Analysis	Test.Replicate_count	Result.Name	Result.Entry	
2	!D44374-3	ICPMS_BIOL	1	Li	0.67	
3	!D44374-3	ICPMS_BIOL	1	Be	<0.1	
4	!D44374-3	ICPMS_BIOL	1	B	180	
5	!D44374-3	ICPMS_BIOL	1	Mg	6600	
6	!D44374-3	ICPMS_BIOL	1	Ca	11000	
7	!D44374-3	ICPMS_BIOL	1	Rb	24.1	
8	!D44374-3	ICPMS_BIOL	1	Sr	670	
9	!D44374-3	ICPMS_BIOL	1	Mo	0.195	
10	!D44374-3	ICPMS_BIOL	1	Ag	<0.05	
11	!D44374-3	ICPMS_BIOL	1	Cd	4.14	
12	!D44374-3	ICPMS_BIOL	1	Sn	<0.5	
13	!D44374-3	ICPMS_BIOL	1	Sb	<0.1	
14	!D44374-3	ICPMS_BIOL	1	Cs	<0.05	
15	!D44374-3	ICPMS_BIOL	1	Ba	7.4	
16	!D44374-3	ICPMS_BIOL	1	Hg	<0.05	
17	!D44374-3	ICPMS_BIOL	1	Tl	<0.1	
18	!D44374-3	ICPMS_BIOL	1	Pb	11.8	
19	!D44374-3	ICPMS_BIOL	1	Bi	<0.05	
20	!D44374-3	ICPMS_BIOL	1	U	0.236	
21	!D44374-3	ICPMS_BIOL	1	Na	34000	
22	!D44374-3	ICPMS_BIOL	1	Al	82	
23	!D44374-3	ICPMS_BIOL	1	P	9900	
24	!D44374-3	ICPMS_BIOL	1	S	20000	
25	!D44374-3	ICPMS_BIOL	1	K	64000	
26	!D44374-3	ICPMS_BIOL	1	V	0.809	
27	!D44374-3	ICPMS_BIOL	1	Cr	2.84	
28	!D44374-3	ICPMS_BIOL	1	Fe	190	
29	!D44374-3	ICPMS_BIOL	1	Mn	13	
30	!D44374-3	ICPMS_BIOL	1	Co	1.13	
31	!D44374-3	ICPMS_BIOL	1	Ni	2.98	
32	!D44374-3	ICPMS_BIOL	1	Cu	1.63	

11 10 04 biologicals

<END>