

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.

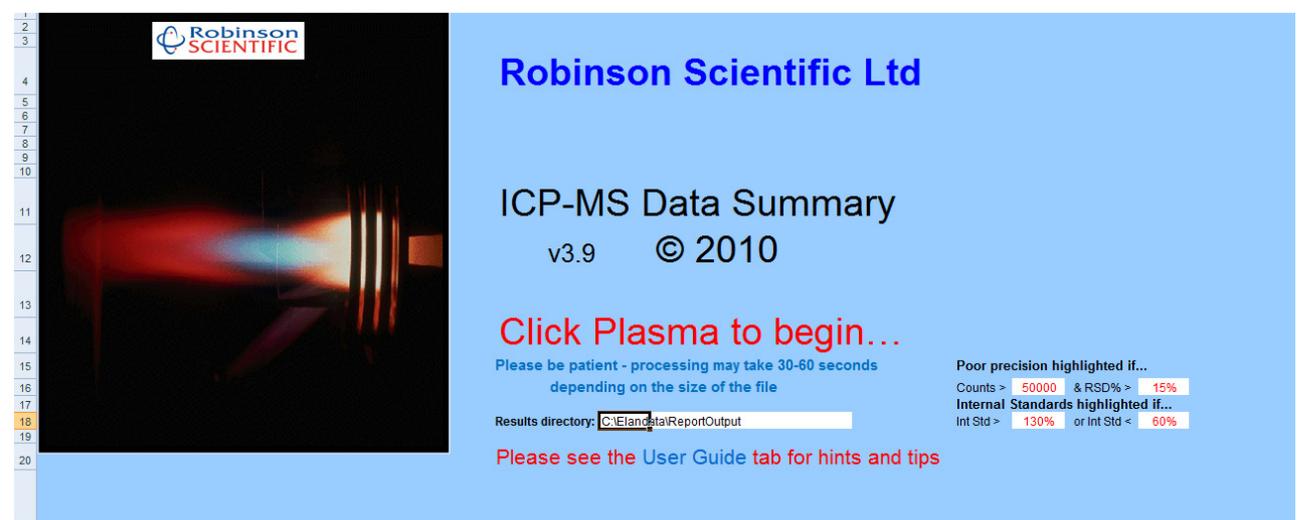
ICP-MS Data Processing Software

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:



Robinson Scientific Ltd

ICP-MS Data Summary
v3.9 © 2010

Click Plasma to begin...

Please be patient - processing may take 30-60 seconds depending on the size of the file

Results directory: C:\Elands\ata\ReportOutput

Poor precision highlighted if...
Counts > 50000 & RSD% > 15%

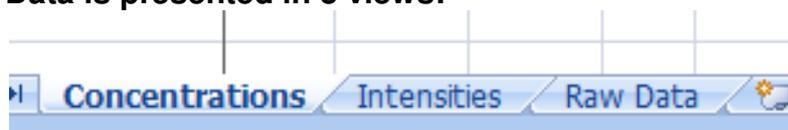
Internal Standards highlighted if...
Int Std > 130% or Int Std < 60%

Please see the User Guide tab for hints and tips

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.
- NB: 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:

	GaX 69	MgX 24	CaX 43	VX 51	CrX 52	FeX 54	FeX 56	MnX 55	CoX 59	NiX 58	NiX 60	CuX 63	CuX 65	ZnX 66	ZnX 68	GaX 71	AsX 75	SeX 78	SeX 82	MoX 98	TeX 125	AsX015 75	SeX015 78	SeX015 82	GaX015 69	Al 27	Sc 45	Mn 55				
4 Blank	100															100					100				100							
5 Standard 1	98	50.00	500.00	5.00	5.00	50.00	50.00	5.00	5.00	5.00	5.00	5.00	50.00	50.00	96	5.00	10.00	10.00	5.00		101	5.00	10.00	10.00	100	5.00	10.00	10.00	102	5.00	98	5.00
6 Rinse Blank1-Waters	98	1.82	-8.95	0.00	0.03	-0.29	0.13	0.00	-0.01	0.01	-0.02	0.00	-0.01	-0.01	-0.20	96	0.00	0.06	0.05	0.09		99	0.00	0.06	0.03	100	-0.02	101	0.00			
7 Rinse Blank2-Waters	97	1.18	16.18	-0.01	0.01	-0.31	0.08	0.00	-0.01	0.01	-0.02	0.00	-0.01	-0.01	-0.12	97	0.00	0.02	0.00	0.02		98	0.00	0.00	0.03	99	0.02	100	0.00			
8 Sample 10x diln	97	88874.16	38714.38	4.57	0.72	1.91	3.26	0.15	0.11	0.09	0.46	0.06	1.23	-0.09	-0.45	95	0.64	0.02	59.70	1.21		99	0.30	0.10	73.23	102	-0.07	104	0.08			
9 Sample 10x diln	98	83576.95	35297.11	4.27	0.66	1.87	2.87	0.14	0.07	0.09	0.36	0.11	1.20	-0.08	-0.50	98	0.59	0.05	58.58	1.20		102	0.32	0.11	73.05	99	-0.08	104	0.08			
10 Sample 10x diln	96	88554.22	37250.39	4.54	0.74	2.23	3.06	0.14	0.12	0.11	0.38	0.21	1.37	-0.07	-0.46	97	0.63	0.04	58.86	1.20		100	0.33	0.11	75.07	97	-0.05	102	0.08			
11 Rinse Blank3-Waters	99	23.60	7.42	0.18	0.05	-0.37	0.02	-0.01	-0.01	-0.05	0.03	0.02	0.05	-0.15	98	0.00	0.00	0.02	0.02		99	0.00	0.00	0.06	101	0.01	92	0.00				
12 Sample 10x diln	98	91523.81	39418.35	4.92	0.76	2.82	3.65	0.33	0.13	0.12	0.45	0.24	1.33	0.13	-0.13	97	0.70	0.05	59.84	1.24		97	0.37	0.14	77.51	99	0.20	104	0.18			
13 Sample 10x diln	97	88508.77	38206.77	4.64	0.77	2.48	3.46	0.29	0.11	0.11	0.42	0.37	1.29	0.14	-0.21	95	0.67	0.05	58.07	1.26		98	0.37	0.10	73.88	98	0.42	94	0.26			
14 Sample 10x diln	95	89305.01	38343.45	4.66	0.73	2.48	3.39	0.32	0.11	0.12	0.47	0.46	1.43	0.15	-0.18	97	0.80	0.06	60.49	1.37		99	0.35	0.12	75.81	99	0.31	102	0.22			
15 Rinse Blank7-Waters	96	50.76	21.55	0.18	0.06	-0.40	0.00	-0.01	-0.02	0.00	0.01	0.07	0.04	0.06	-0.23	98	0.00	0.00	0.06	0.03		100	0.00	0.00	0.08	101	0.00	93	-0.01			
16 Sppb Std Ck2-Waters	98	59.03	471.19	4.83	4.84	48.76	47.77	4.83	4.90	4.65	5.05	4.89	4.80	49.91	50.57	99	5.08	9.96	9.92	5.00		99	4.93	10.09	9.82	99	4.89	95	4.66			

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	37250.39	4.54	0.74
11	Rinse Blank3-Waters	99	23.60	7.42	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	Sppb Std Ck2-Waters	98	59.03	471.19	4.83	4.84

Intensities View:

	GaX 69	CX 12	CIX 35	MgX 24	CaX 43	VX 51	CrX 52	FeX 54	FeX 56	MnX 55	CoX 59	NiX 58	NiX 60	CuX 63	CuX 65	ZnX 66	ZnX 68	GaX 71	AsX 75	SeX 78	SeX 82	MoX 98	TeX 125	AsX015 75	SeX015 78	SeX015 82	GaX015 69	
4 Blank	6306455	2022546	4561	2157	769	335	376	381	1418	145	603	32	271	146	61	118	626	3566965	4	1	3	9	40061	6	6	6	4	4003922
5 Standard 1	5434944	2018996	3872	33428	2323	10977	9569	7976	129088	15009	14563	8348	3619	7775	3751	22684	16376	3056093	1660	1882	820	4374	38641	3727	2089	878	3742222	
6 Rinse Blank1-Waters	5206894	1908862	3525	2881	805	269	365	272	1500	125	468	46	212	115	46	95	454	2939646	4	12	7	84	37606	7	17	6	3700489	
7 Rinse Blank2-Waters	5165395	1965413	3474	2458	675	258	325	265	1348	129	459	40	210	124	41	91	471	2897510	4	4	3	27	37206	4	6	6	3684275	
8 Sample 10x diln	4979907	1905267	11962	51428748	118742	9215	1521	567	8769	532	766	168	500	204	883	50	362	2808190	153	4	3480	758	27569	223	26	6164	3589922	
9 Sample 10x diln	5097247	1492515	11534	50105050	112225	8934	1465	582	8131	505	682	169	452	282	890	61	360	2902287	143	7	3417	755	27587	235	27	6212	3634356	
10 Sample 10x diln	4835670	1575417	11452	50414996	112245	9013	1525	602	8143	498	758	189	445	396	962	60	352	2755156	152	6	3445	756	27683	240	27	6231	3547104	
11 Rinse Blank3-Waters	4630978	1730585	3190	50001	12375	567	359	231	1082	92	430	45	169	150	60	104	418	2614868	3	1	4	26	39899	5	6	8	3281597	
12 Sample 10x diln	4611214	1532213	11342	49338673	112632	9227	1471	648	9007	938	754	191	456	416	888	138	423	2609267	163	8	3357	751	26536	258	31	6202	3420011	
13 Sample 10x diln	4837854	1556281	11451	4996399	114411	9128	1565	631	9006	883	745	194	460	624	898	147	419	2734907	162	7	3386	791	27568	273	26	6225	3606096	
14 Sample 10x diln	4761217	1516210	11558	50940789	115939	9254	1517	638	8927	963	757	204	501	751	1002	152	433	2760723	186	9	3430	837	26819	256	28	6295	3548795	
15 Rinse Blank7-Waters	4541374	1718296	3231	28386	612	570	361	222	1021	78	392	29	198	200	68	109	389	2561665	3	0	7	28	32373	5	6	9	3207446	
16 Sppb Std Ck2-Waters	4298789	1599147	2698	31240	1779	8485	7400	6221	98585	11588	11415	6198	2917	6077	2877	18090	13226	2440937	1362	1513	657	3531	31192	3005	1724	706	3058406	

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\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								

<END>