# 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.

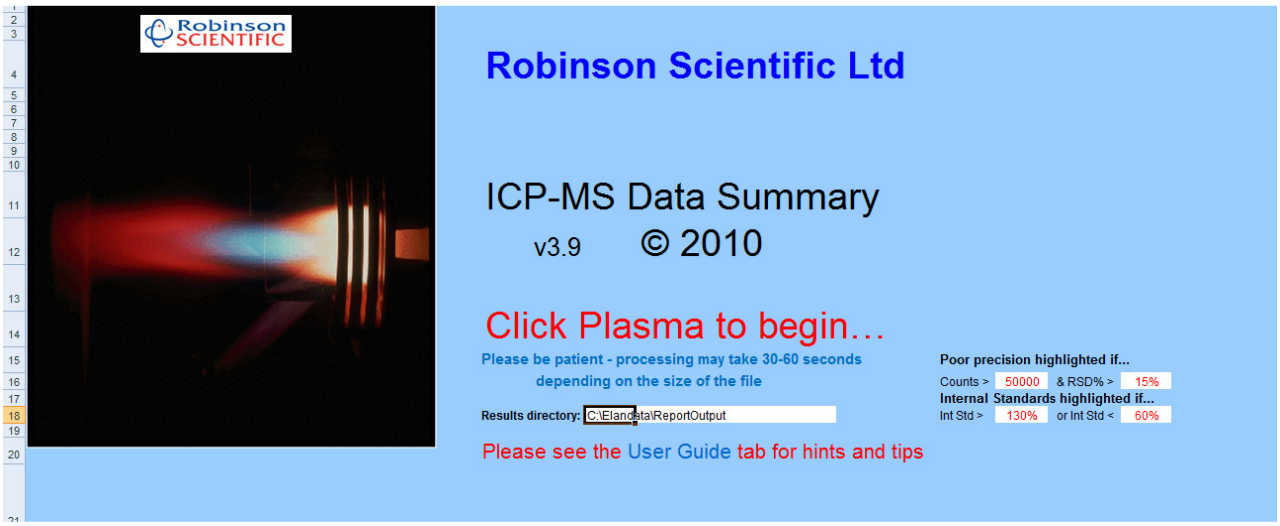
## ICP-MS Data Processing Software

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.

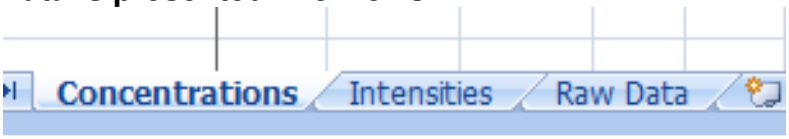
Main screen:



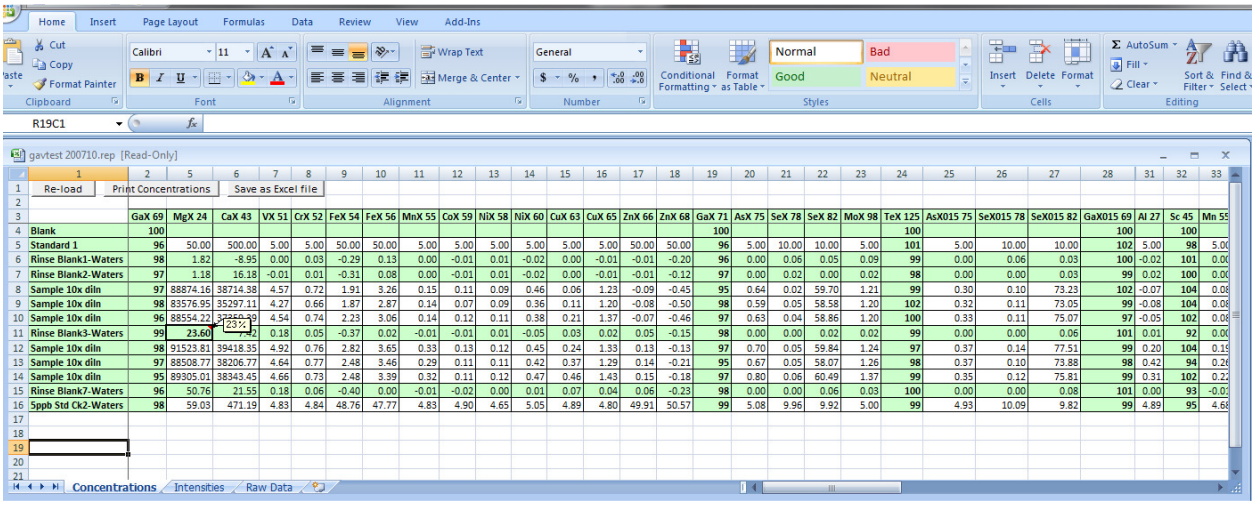
**Notes & Comments from the User Guide:**

- 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.
- 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" botton 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

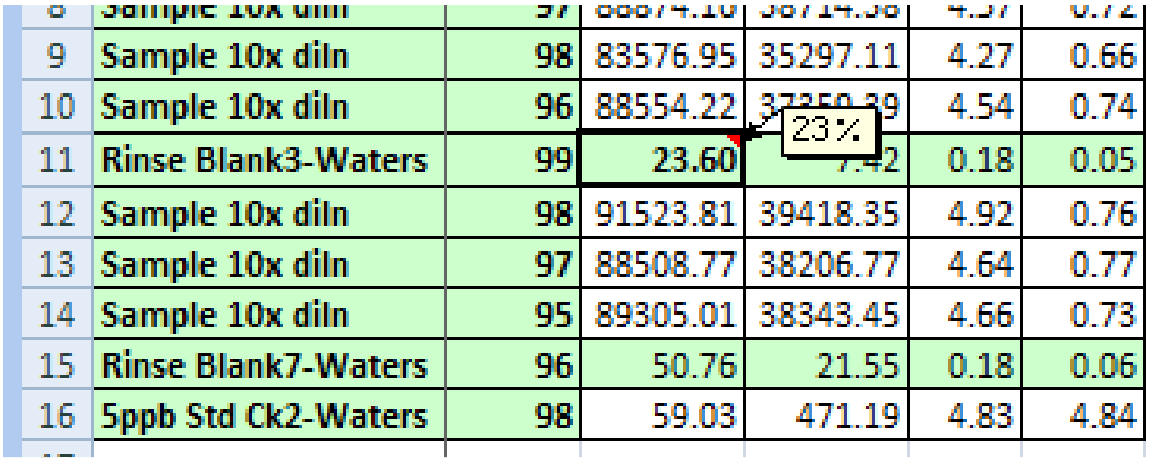
**Data is presented in 3 views:**



**Concentrations** View:

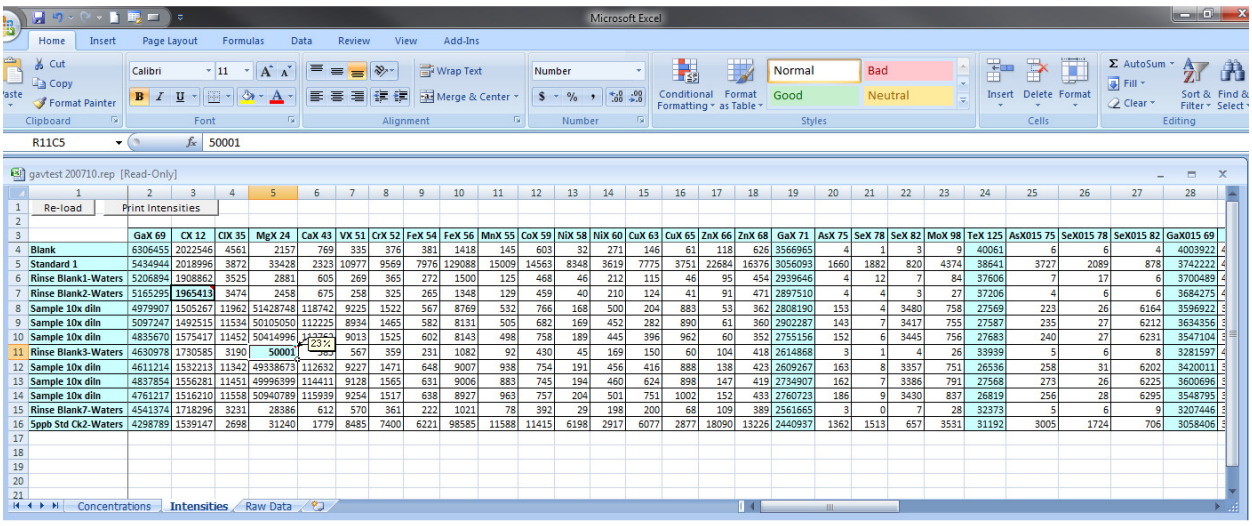


Note the highlighted poor precision – in this case due to carry-over from a high sample:



| | | | | | | |
|---|---|---|---|---|---|---|
| 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:



**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

<END>