Transcription free integration with the Agilent 7700 ICP-MS \blacksquare CSO S

Mass Spectrometer and MassHunter software



laboratory systems integration

Links 4 LIMS



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Background

The popularity of trace element analysis by Inductively Coupled Plasma Mass Spectrometry continues to grow, driven by a number of factors, including:

- Improvements in instrumentation (e.g. ability to run difficult sample types directly rather than with pre-treatment)
- Improved sample preparation and introduction systems (e.g. laser ablation for solids, faster, more sophisticated autosamplers, IC or LC integration for speciation studies, and ability to introduce smaller samples)
- Ability to undertake analysis on novel materials (e.g. nanoparticle analysis)
- An increase in the demand for specific test methods (e.g. trace elements in soils prompted by an increase in the number of land surveys performed)
- New regulations requiring decreased detection limits.

Whichever trend is relevant to individual laboratories, the net result is that not only has the amount of data generated increased but so has the administration burden on analysts. Not just to physically transcribe information but also the effort required to interpret and review results before releasing them.

Transcription free operation

This poster shows how you can use CSols Links for LIMS and AqcTools software to maximize your investment in the Agilent 7700 (or 7500, 7900 or 8800) ICP-MS instrument to streamline both instrument setup and results handling, so as to reduce turnaround times and improve results quality.

Instrument setup and loading

Whether your laboratory operates with worklists (lists of samples requiring a specific test method) or in an ad-hoc way with samples as they arrive on the bench, setting up a batch run electronically can save precious time and remove errors. If a LIMS or LIS system is used it's possible to extract and read a LIMS generated worklist or to ask electronically for all outstanding samples. For ad-hoc testing, barcode reading can verify that the sample is already registered and has the correct tests assigned. Here (Figure 1) Links for LIMS has extracted a set of samples for a specific run together with associated sample biographical data, and has inserted all the necessary controls. This list can be re-ordered to move highly concentrated samples or ones from a specific location before setting up the instrument. Once saved this run can be opened directly in MassHunter.

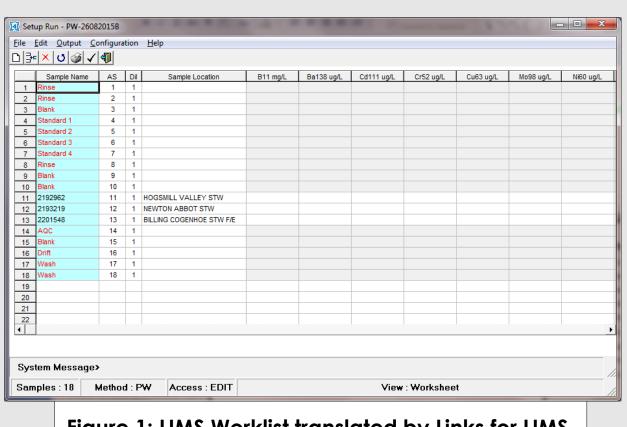
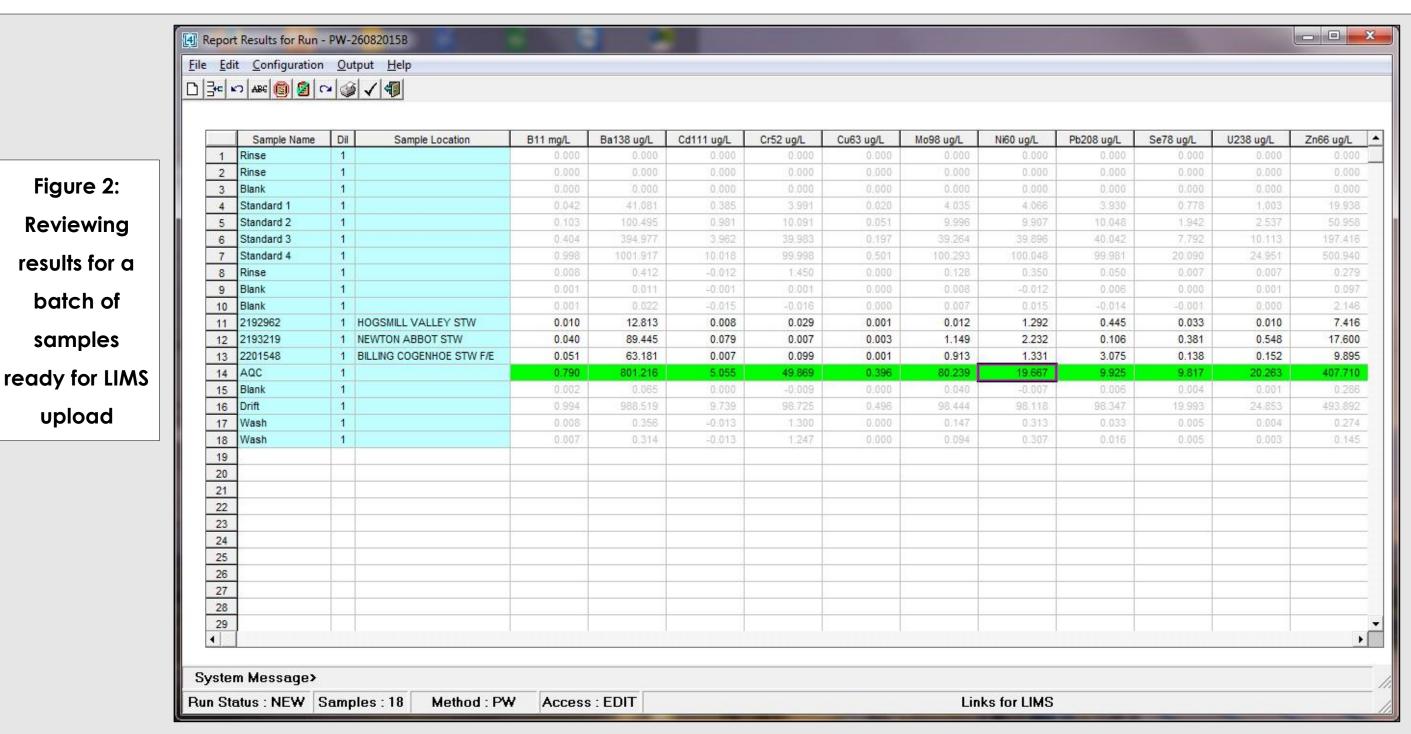


Figure 1: LIMS Worklist translated by Links for LIMS



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		CalBlk	Rinse		1	Sample2.d					
		CalBlk	Blank		1	Sample3.d		_			
		CalStd	Standard 1		2	Sample4.d	Sample4.d				
		CalStd	Standard 2		3	Sample5.d	Level 2		0		
		CalStd	Standard 3		4	Sample6.d	Level 3				
		CalStd	1000000		5	Sample7.d		Level 4			
		CalBlk	Rinse		1	Sample8.d					
		CalBlk	Blank		1	Sample9.d					
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ŧ.		QC1	AQC		4101	Sample14.d			50		
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Figure 3: Batch run created by Links for LIMS, opened in MassHunter

Extracting results

Extracting or reporting results from MassHunter can be streamlined using MassHunter scripts. These can be launched directly from the MassHunter Offline Data analysis module menu, saving time and eliminating any unnecessary user dialog. Links for LIMS in turn can be launched directly from the script or run at a separate PC workstation in the laboratory. See Figure 4.

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1			002SMPL.d	26/08/2015 13:48:5	5	Sample		Rinse						
2			003SMPL.d	26/08/2015 13:52:10		Sample		Rinse				,		
3			004CALB.d	26/08/2015 13:55:2	5	CalBlk	1	Blank	0	.000	N/A	0.000	N/A	
4			005CALS.d	26/08/2015 13:58:5	0	CalStd	2	Standard 1	0	.042	0.5	3.991	4.9	
5			006CALS.d	26/08/2015 14:02:1	5	CalStd	3	Standard 2	0	103	0.5	10.091	1.5	
6			007CALS.d	26/08/2015 14:05:3	9	CalStd	4	Standard 3	0	404	0.6	39.983	1.4	
7	20 10		008CALS.d	26/08/2015 14:09:04	4	CalStd	5	Standard 4	0	998	0.1	99.998	1.2	

Figure 4: MassHunter script being launched

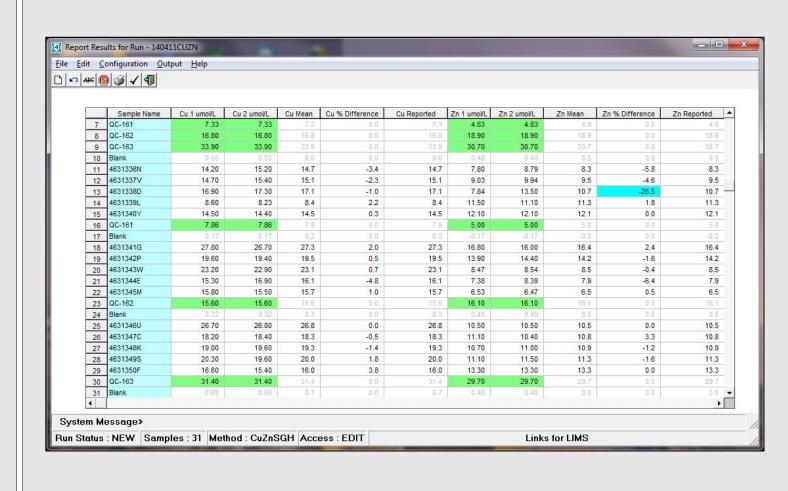


Figure 5: Results complete with duplicate calculations

Results Reporting

Rather than introducing further electronic transcription through, for example Microsoft Excel, we believe that analysts would rather deal with the results as soon as possible. Links for LIMS then has everything that is needed. From flagging and formatting results, to handling weights and dilution factors, to calculations, through to holding of all the necessary data to allow a direct upload to LIMS without leaving the software.

Figures 2 & 5 show some example result configurations.

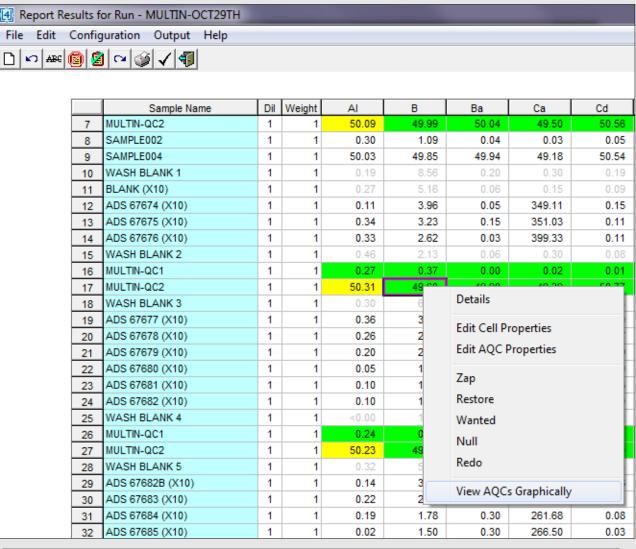


Figure 6. AQC Charts can be launched from Links for LIMS

Viewing AQC Results

AQCs are immediately flagged using colour coding. Historical AQCs can also be viewed using the AqcTools software. This will include all limit and trend exceptions.

Summary

Links for LIMS is reducing the administration effort on thousands of instruments around the world. On an Agilent ICP-MS with MassHunter Links for LIMS can eliminate data transcription saving between 3% & 5% errors compared to manual processes, can save many man hours of effort per run in the immediate post processing of results, and allows analysts to react immediately to AQC exceptions.

Further Information

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