

# Transcription free integration with the Agilent 7700 ICP-MS CSols

## Mass Spectrometer and MassHunter software

laboratory systems integration

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Links  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.

Sample Name	AS	DI	Sample Location	B11 mg/L	Ba138 ug/L	Cd111 ug/L	Cr52 ug/L	Cu63 ug/L	Mo98 ug/L	Nb93 ug/L
1 Rinse	1			0.000	0.000	0.000	0.000	0.000	0.000	0.000
2 Rinse	1			0.000	0.000	0.000	0.000	0.000	0.000	0.000
3 Blank	1			0.000	0.000	0.000	0.000	0.000	0.000	0.000
4 Standard 1	1			0.042	41.961	0.981	3.991	0.020	4.635	4.966
5 Standard 2	1			0.103	100.495	0.981	10.091	0.051	9.996	9.907
6 Standard 3	1			0.404	394.977	3.982	39.993	0.197	39.264	39.896
7 Standard 4	1			0.998	1001.917	10.018	99.998	0.501	100.293	100.048
8 Rinse	1			0.008	0.412	-0.012	1.450	0.000	0.128	0.350
9 Blank	1			0.001	0.011	-0.001	0.001	0.000	0.008	-0.012
10 Blank	1			0.001	0.022	-0.015	-0.016	0.000	0.007	0.015
11 2192962	1		HOGSMILL VALLEY STW	0.010	12.813	0.008	0.029	0.001	0.012	1.292
12 2193219	1		NEWTON ABBOT STW	0.040	89.445	0.079	0.007	0.003	1.149	2.232
13 2201548	1		BILLING COGENHOE STW F/E	0.051	63.181	0.007	0.099	0.001	0.913	1.331
14 AQC	1			0.790	801.216	5.955	49.969	0.396	90.238	19.967
15 Blank	1			0.002	0.055	0.000	-0.009	0.000	0.040	-0.007
16 Drift	1			0.994	988.519	9.739	98.725	0.496	98.444	98.118
17 Wash	1			0.008	0.358	-0.013	1.300	0.000	0.147	0.313
18 Wash	1			0.007	0.314	-0.013	1.247	0.000	0.094	0.307

Figure 1: LIMS Worklist translated by Links for LIMS

Figure 2: Reviewing results for a batch of samples ready for LIMS upload

Sample Name	DI	Sample Location	B11 mg/L	Ba138 ug/L	Cd111 ug/L	Cr52 ug/L	Cu63 ug/L	Mo98 ug/L	Nb93 ug/L	Pb208 ug/L	Se78 ug/L	U238 ug/L	Zn66 ug/L
1 Rinse	1		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2 Rinse	1		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
3 Blank	1		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
4 Standard 1	1		0.042	41.961	0.981	3.991	0.020	4.635	4.966	3.930	9.778	1.003	19.938
5 Standard 2	1		0.103	100.495	0.981	10.091	0.051	9.996	9.907	10.848	1.942	2.537	50.958
6 Standard 3	1		0.404	394.977	3.982	39.993	0.197	39.264	39.896	40.042	7.792	10.113	197.416
7 Standard 4	1		0.998	1001.917	10.018	99.998	0.501	100.293	100.048	99.981	20.090	24.961	500.940
8 Rinse	1		0.008	0.412	-0.012	1.450	0.000	0.128	0.350	0.000	0.007	0.007	0.279
9 Blank	1		0.001	0.011	-0.001	0.001	0.000	0.008	-0.012	0.000	0.000	0.001	0.097
10 Blank	1		0.001	0.022	-0.015	-0.016	0.000	0.007	0.015	-0.014	-0.001	0.000	2.148
11 2192962	1		0.010	12.813	0.008	0.029	0.001	0.012	1.292	0.445	0.033	0.010	7.416
12 2193219	1		0.040	89.445	0.079	0.007	0.003	1.149	2.232	0.106	0.381	0.548	17.600
13 2201548	1		0.051	63.181	0.007	0.099	0.001	0.913	1.331	3.075	0.138	0.152	9.895
14 AQC	1		0.790	801.216	5.955	49.969	0.396	90.238	19.967	9.925	9.817	20.263	407.710
15 Blank	1		0.002	0.055	0.000	-0.009	0.000	0.040	-0.007	0.006	0.004	0.001	0.296
16 Drift	1		0.994	988.519	9.739	98.725	0.496	98.444	98.118	98.347	19.993	24.853	493.892
17 Wash	1		0.008	0.358	-0.013	1.300	0.000	0.147	0.313	0.033	0.005	0.004	0.274
18 Wash	1		0.007	0.314	-0.013	1.247	0.000	0.094	0.307	0.016	0.005	0.003	0.145

Step	Sample Type	Sample Name	Comment	Vial#	File Name	Replicates	Level	Dilution
1	CalBlk	Rinse		1	Sample1.d			
2	CalBlk	Rinse		1	Sample2.d			
3	CalBlk	Blank		1	Sample3.d			
4	CalStd	Standard 1		2	Sample4.d		Level 1	
5	CalStd	Standard 2		3	Sample5.d		Level 2	
6	CalStd	Standard 3		4	Sample6.d		Level 3	
7	CalStd	Standard 4		5	Sample7.d		Level 4	
8	CalBlk	Rinse		1	Sample8.d			
9	CalBlk	Blank		1	Sample9.d			
10	CalBlk	Blank		1	Sample10.d			
11	Sample	2192962		1101	Sample11.d			
12	Sample	2193219		1102	Sample12.d			
13	Sample	2201548		1103	Sample13.d			
14	AQC			4101	Sample14.d			
15	CalBlk	Blank		1	Sample15.d			

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.

File	View	Process	DA Method	Report	Tools	Global Help
002SMP.d	26/08/2015 13:48:55	Sample	Rinse			
003SMP.d	26/08/2015 13:52:10	Sample	Rinse			
004CALB.d	26/08/2015 13:55:25	CalBlk	Blank	0.000	N/A	0.000
005CALSD	26/08/2015 13:58:50	CalStd	Standard 1	0.042	0.5	3.991
006CALSD	26/08/2015 14:02:15	CalStd	Standard 2	0.103	0.5	10.091
007CALSD	26/08/2015 14:05:39	CalStd	Standard 3	0.404	0.6	39.983
008CALSD	26/08/2015 14:09:04	CalStd	Standard 4	0.998	0.1	99.998

Figure 4: MassHunter script being launched

Sample Name	Cu 1 ug/L	Cu 2 ug/L	Cu Mean	Cu % Difference	Cu Reported	Zn 1 ug/L	Zn 2 ug/L	Zn Mean	Zn % Difference	Zn Reported
7 QC-H1	7.03	7.33	7.18	4.88	4.93	18.90	18.90	18.90	0.0	18.9
8 QC-H2	16.90	16.90	16.90	0.0	16.9	16.90	16.90	16.90	0.0	16.9
9 QC-H3	33.80	33.80	33.80	0.0	33.8	33.80	33.80	33.80	0.0	33.8
10 Blank	0.00	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.0	0.0
11 4013380	14.20	15.20	14.7	-3.4	14.7	7.80	8.79	8.3	-5.8	8.3
12 4013379	14.10	15.40	15.1	2.3	15.1	9.03	9.94	9.5	-4.0	9.5
13 4013380	16.90	17.30	17.1	-1.0	17.1	7.84	13.50	10.7	-28.5	10.7
14 4013380	8.60	8.23	8.4	2.2	8.4	11.50	11.50	11.5	0.0	11.5
15 4013407	14.60	14.40	14.5	0.3	14.5	12.10	12.10	12.1	0.0	12.1
16 QC-H1	7.96	7.96	7.96	0.0	7.9	5.00	5.00	5.0	0.0	5.0
17 Blank	0.00	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.0	0.0
18 4013410	27.80	26.70	27.3	2.8	27.3	16.80	16.80	16.8	0.0	16.8
19 4013420	19.60	19.40	19.5	0.5	19.5	13.90	14.40	14.2	-1.8	14.2
20 4013430	23.20	22.90	23.1	0.7	23.1	8.47	8.54	8.5	-0.4	8.5
21 4013440	15.30	16.90	16.1	-4.8	16.1	7.80	8.39	7.9	-4.4	7.9
22 4013450	15.80	15.50	15.7	1.0	15.7	6.53	6.47	6.5	0.0	6.5
23 QC-H2	15.60	15.60	15.60	0.0	15.6	16.16	16.16	16.1	0.0	16.1
24 Blank	0.00	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.0	0.0
25 4013460	26.70	26.80	26.8	0.0	26.8	10.50	10.50	10.5	0.0	10.5
26 4013470	18.20	18.40	18.3	-0.5	18.3	11.10	10.40	10.8	3.3	10.8
27 4013480	19.00	19.60	19.3	-1.4	19.3	10.70	11.00	10.9	-1.2	10.9
28 4013490	20.30	19.60	20.0	1.8	20.0	11.10	11.50	11.3	-1.6	11.3
29 4013500	16.60	15.40	16.0	3.8	16.0	13.30	13.30	13.3	0.0	13.3
30 QC-H3	31.60	31.60	31.60	0.0	31.6	20.90	20.90	20.9	0.0	20.9
31 Blank	0.00	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.0	0.0

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.

Sample Name	DI	Weight	AI	B	Ba	Ca	Cd
7 MULTIN-QC2	1	1	50.09	49.99	50.04	49.50	50.56
8 SAMPLE002	1	1	0.30	1.09	0.04	0.03	0.05
9 SAMPLE004	1	1	50.03	49.85	49.94	49.18	50.54
10 WASH BLANK 1	1	1	0.19	0.56	0.20	0.30	0.19
11 BLANK (X10)	1	1	0.27	5.16	0.06	0.15	0.09
12 ADS 67674 (X10)	1	1	0.11	3.96	0.05	349.11	0.15
13 ADS 67675 (X10)	1	1	0.34	3.23	0.15	351.03	0.11
14 ADS 67676 (X10)	1	1	0.33	2.62	0.03	399.33	0.11
15 WASH BLANK 2	1	1	0.19	0.56	0.20	0.30	0.19
16 MULTIN-QC1	1	1	50.31	49.99	50.04	49.50	50.56
17 MULTIN-QC2	1	1	50.31	49.99	50.04	49.50	50.56
18 WASH BLANK 3	1	1	0.19	0.56	0.20	0.30	0.19
19 ADS 67677 (X10)	1	1	0.36	3.23			