

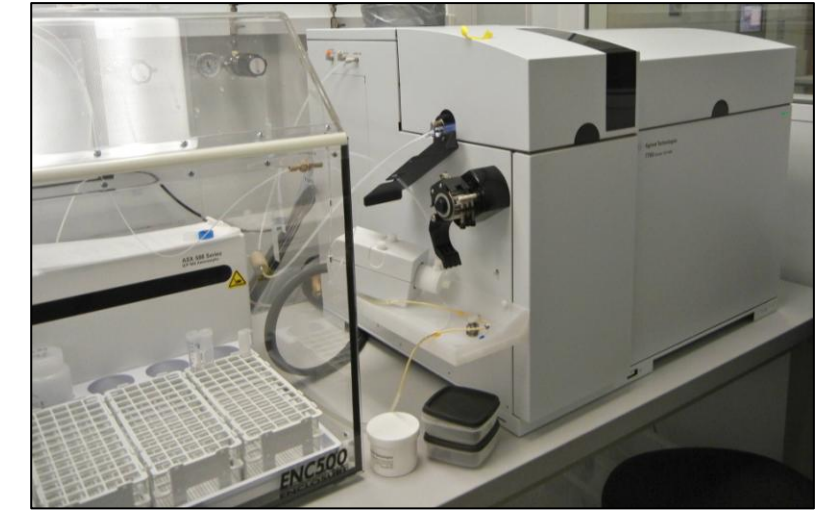
# Transcription free integration with the Agilent 7700 ICP-MS CSols

## 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 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	Nb60 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	41.081	0.385	3.991	0.020	4.035	4.068
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	3.962	39.983	0.197	39.264	39.086
7 Standard 4	1			0.998	1001.917	10.018	99.998	0.501	100.293	100.046
8 Rinse	1			0.008	0.412	-0.012	1.450	0.000	0.128	0.358
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	99.445	0.079	0.007	0.003	1.149	2.232
13 2201548	1		BILLING COGENHOE STW FE	0.051	63.181	0.007	0.099	0.001	0.913	1.331
14 AQC	1			0.790	801.216	7.345	49.969	0.396	80.239	19.067
15 Blank	1			0.000	0.000	0.000	0.000	0.000	0.000	0.000
16 Drift	1			0.994	998.519	9.739	98.725	0.498	98.444	98.118
17 Wash	1			0.008	0.356	-0.013	1.300	0.000	0.147	0.313
18 Wash	1			0.007	0.314	-0.013	1.347	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	Nb60 ug/L	Ph208 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	41.081	0.385	3.991	0.020	4.035	4.068	3.930	0.778	1.003	19.938
5 Standard 2	1		0.103	100.495	0.981	10.091	0.051	9.996	9.907	10.046	1.942	2.537	50.958
6 Standard 3	1		0.404	394.977	3.962	39.983	0.197	39.264	39.086	40.042	7.752	10.113	197.416
7 Standard 4	1		0.998	1001.917	10.018	99.998	0.501	100.293	100.046	99.981	20.090	24.951	500.940
8 Rinse	1		0.008	0.412	-0.012	1.450	0.000	0.128	0.358	0.950	0.007	0.007	0.279
9 Blank	1		0.001	0.011	-0.001	0.001	0.000	0.008	-0.012	0.008	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	-0.000	0.000	2.146
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	99.445	0.079	0.007	0.003	1.149	2.232	0.106	0.381	0.548	17.000
13 2201548	1		0.051	63.181	0.007	0.099	0.001	0.913	1.331	3.075	0.138	0.152	9.985
14 AQC	1		0.790	801.216	7.345	49.969	0.396	80.239	19.067	0.925	3.017	21.263	407.710
15 Blank	1		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
16 Drift	1		0.994	998.519	9.739	98.725	0.498	98.444	98.118	98.347	19.993	24.853	493.692
17 Wash	1		0.008	0.356	-0.013	1.300	0.000	0.147	0.313	0.933	0.005	0.004	0.274
18 Wash	1		0.007	0.314	-0.013	1.347	0.000	0.094	0.307	0.916	0.005	0.003	0.145

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.

Sample Name	AS	DI	Sample Location	B11 mg/L	Ba138 ug/L	Cd111 ug/L	Cr52 ug/L	Cu63 ug/L	Mo98 ug/L	Nb60 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	41.081	0.385	3.991	0.020	4.035	4.068
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	3.962	39.983	0.197	39.264	39.086
7 Standard 4	1			0.998	1001.917	10.018	99.998	0.501	100.293	100.046

Figure 4: MassHunter script being launched

Sample Name	DI	Sample Location	B11 mg/L	Ba138 ug/L	Cd111 ug/L	Cr52 ug/L	Cu63 ug/L	Mo98 ug/L	Nb60 ug/L	Ph208 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	41.081	0.385	3.991	0.020	4.035	4.068	3.930	0.778	1.003	19.938
5 Standard 2	1		0.103	100.495	0.981	10.091	0.051	9.996	9.907	10.046	1.942	2.537	50.958
6 Standard 3	1		0.404	394.977	3.962	39.983	0.197	39.264	39.086	40.042	7.752	10.113	197.416
7 Standard 4	1		0.998	1001.917	10.018	99.998	0.501	100.293	100.046	99.981	20.090	24.951	500.940
8 Rinse	1		0.008	0.412	-0.012	1.450	0.000	0.128	0.358	0.950	0.007	0.007	0.279
9 Blank	1		0.001	0.011	-0.001	0.001	0.000	0.008	-0.012	0.008	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	-0.000	0.000	2.146
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	99.445	0.079	0.007	0.003	1.149	2.232	0.106	0.381	0.548	17.000
13 2201548	1		0.051	63.181	0.007	0.099	0.001	0.913	1.331	3.075	0.138	0.152	9.985
14 AQC	1		0.790	801.216	7.345	49.969	0.396	80.239	19.067	0.925	3.017	21.263	407.710
15 Blank	1		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
16 Drift	1		0.994	998.519	9.739	98.725	0.498	98.444	98.118	98.347	19.993	24.853	493.692
17 Wash	1		0.008	0.356	-0.013	1.300	0.000	0.147	0.313	0.933	0.005	0.004	0.274
18 Wash	1		0.007	0.314	-0.013	1.347	0.000	0.094	0.307	0.916	0.005	0.003	0.145

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 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	50.30	49.99	55.04	49.50	53.36
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	0.09	0.20	0.30	0.13
11 BLANK (X10)	1	1	0.27	0.10	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	0.46	0.13	0.06	0.30	0.00
16 MULTIN-QC1	1	1	0.27	0.37	0.00	0.02	0.01
17 MULTIN-QC2	1	1	50.31	49.99	55.04	49.50	53.36
18 WASH BLANK 3	1	1	0.30	1.09	0.04	0.03	0.05
19 ADS 67677 (X10)	1	1	0.36	3.23	0.15	351.03	0.11
20 ADS 67678 (X10)	1	1	0.26	2.62	0.03	399.33	0.11
21 ADS 67679 (X10)	1	1	0.20	2.00	0.02	200.00	0.02
22 ADS 67680 (X10)	1	1	0.05	0.05	0.00	0.00	0.00
23 ADS 67681 (X10)	1	1	0.10	1.00	0.01	0.01	0.01
24 ADS 67682 (X10)	1	1	0.10	1.00	0.01	0.01	0.01
25 WASH BLANK 4	1	1	-0.00	0.00	0.00	0.00	0.00
26 MULTIN-QC1	1	1	0.27	0.37	0.00	0.02	0.01
27 MULTIN-QC2	1	1	50.31	49.99	55.04	49.50	53.36
28 WASH BLANK 5	1	1	0.30	1.09	0.04	0.03	0.05
29 ADS 67682B (X10)	1	1	0.14	1.40	0.01	0.01	0.01
30 ADS 67683 (X10)	1	1	0.22	2.20	0.01	0.01	0.01
31 ADS 67684 (X10)	1	1	0.19	1.78	0.30	261.68	0.08
32 ADS 67685 (X10)	1	1	0.02	1.50			