

Simple batch processing of GC-MS and LC-MS/MS results for LIMS upload from MassHunter software

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Links **4** LIMS



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Background

MassHunter is a very powerful software application designed for the control, data capture, data processing and reporting from all of the Agilent GC-MS and LC-MS/MS Mass Spectrometer product ranges. With many test methods generating large numbers of results, (e.g. pesticides in drinking water or drugs of abuse in urine) or where MassHunter post run modules create additional derived data, it is essential that the appropriate capabilities are in place to deal with this data effectively. MassHunter already provides a comprehensive on board reporting capability and related utilities. However it does not always offer the necessary data translation, conversion and alignment facilities required in different laboratories to easily pass suitable data backwards and forwards to systems such as Laboratory Information Management Systems (i.e. LIMS, LIS), Manufacturing systems (e.g. SCADA, ERP, MRPII) or other databases. Moreover while MassHunter also offers a wide range of result validation facilities offering colour coded flags indicating possible instrument errors, it does not offer direct access to historical Analytical Quality Control AQC data to meet the regulatory drive (i.e. ISO17025, ISO15189) to become more responsive to limit or trend AQC exceptions.

Simple batch processing

This poster explains how CSols Links and LIMS software can fully complement the capabilities of MassHunter for all GC-MS & LC-MS/MS analysis, can provide both a flexible modular solution for seamless integration with other IT systems, and offer immediate access to relevant AQC data.

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. Links for LIMS can easily translate many different LIMS worklist formats and merge control samples into a predefined layout (see Figure 1) ready for direct instrument set up.

Sample Name	Anthracene	Fluoranthene	Benzo(b)fluoranthene	Benzo(k)fluoranthene	Benzo(a)pyrene
1 Neat	0.01129	0.01943	0.01176	0.01599	0.01106
2 10ngl std	0.009617	0.00789	0.00168	0.00057	0.00058
3 1ngl std	0.001602	0.001751	0.001137	0.001029	0.001029
4 5ngl std	0.005408	0.005498	0.004995	0.004937	0.005239
5 10ngl std	0.010496	0.010476	0.010777	0.009984	0.010023
6 17.5ngl std	0.019815	0.017887	0.018361	0.017962	0.017502
7 25ngl std	0.027734	0.028517	0.027544	0.027992	0.027185
8 Neat Blank	<-0.00059	<-0.00043	<-0.00092	<-0.00056	<-0.00038
9 AQC YOWOH Extra	0.009446	0.009746	0.009127	0.009036	0.009130
10 547169	<-0.00059	<-0.00039	<-0.00092	<-0.00056	<-0.00038
11 AQC YOWOH	0.009590	0.009567	0.009321	0.009114	0.009234
12 543310	<-0.00059	0.00360	<-0.00092	<-0.00063	<-0.00039
13 543338	<-0.00059	0.00067	<-0.00092	<-0.00063	<-0.00039
14 543381	<-0.00059	0.00086	<-0.00092	<-0.00063	<-0.00039
15 543495	0.00150	0.00550	0.00230	0.00081	0.00120
16 543502	0.00140	0.00350	0.00120	<-0.00063	0.00120
17 543564	0.00210	0.01500	<-0.00092	<-0.00063	<-0.00039
18 551271	0.00060	0.00150	<-0.00092	<-0.00063	<-0.00039
19 543623	0.00170	0.01400	0.01500	0.01100	0.01000
20 543802	<-0.00059	0.01500	<-0.00092	<-0.00063	<-0.00039
21 543915	0.00450	0.02000	0.00110	<-0.00063	<-0.00039
22 543923	0.00110	0.01300	<-0.00092	<-0.00063	<-0.00039
23 543987	<-0.00059	0.00095	<-0.00092	<-0.00063	<-0.00039
24 544105	<-0.00059	0.00780	<-0.00092	<-0.00063	<-0.00039
25 544233	0.00097	0.00980	<-0.00092	<-0.00063	<-0.00039
26 544234	0.00210	0.00560	<-0.00092	<-0.00063	<-0.00039
27 544502	<-0.00059	0.00280	<-0.00092	<-0.00063	<-0.00039
28 AQC YOWOH	0.009241	0.009517	0.009492	0.009217	0.009211
29 553651	<-0.00059	0.00077	<-0.00092	<-0.00063	<-0.00039
30 553652	<-0.00059	0.00078	<-0.00092	<-0.00063	<-0.00039
31 553653	0.00064	0.00072	<-0.00092	<-0.00063	<-0.00039
32 553654	0.00063	0.00073	<-0.00092	<-0.00063	<-0.00039
33 553655	0.00060	0.00078	<-0.00092	<-0.00063	<-0.00039
34 AQC YOWOH	0.009477	0.009143	0.009253	0.009149	0.009270
35 553656	<-0.00059	0.00073	<-0.00092	<-0.00063	<-0.00039
36 553657	<-0.00059	0.00089	<-0.00092	<-0.00063	<-0.00039
37 553658	<-0.00059	0.00100	<-0.00092	<-0.00063	<-0.00039
38 553659	<-0.00059	0.00064	<-0.00092	<-0.00063	<-0.00039
39 553983	<-0.00059	0.00069	<-0.00092	<-0.00063	<-0.00038

Figure 1: Links for LIMS instrument setup

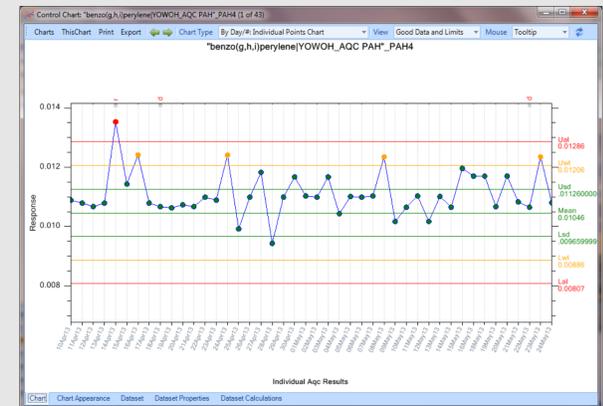
Figure 2: Reviewing results in Links for LIMS

Sample Name	Anthracene	Fluoranthene	Benzo(b)fluoranthene	Benzo(k)fluoranthene	Benzo(a)pyrene	Indeno(1,2,3-cd)pyrene	Benzo(g,h,i)perylene	PAH (total by calculation)
1 Neat	0.01129	0.01943	0.01176	0.01599	0.01106	0.01106	0.01106	0.00000
2 10ngl std	0.009617	0.00789	0.00168	0.00057	0.00058	0.00058	0.00058	0.00000
3 1ngl std	0.001602	0.001751	0.001137	0.001029	0.001029	0.001029	0.001029	0.00000
4 5ngl std	0.005408	0.005498	0.004995	0.004937	0.005239	0.005239	0.005239	0.00000
5 10ngl std	0.010496	0.010476	0.010777	0.009984	0.010023	0.010023	0.010023	0.00000
6 17.5ngl std	0.019815	0.017887	0.018361	0.017962	0.017502	0.017502	0.017502	0.00000
7 25ngl std	0.027734	0.028517	0.027544	0.027992	0.027185	0.027185	0.027185	0.00000
8 Neat Blank	<-0.00059	<-0.00043	<-0.00092	<-0.00056	<-0.00038	<-0.00038	<-0.00038	0.00000
9 AQC YOWOH Extra	0.009446	0.009746	0.009127	0.009036	0.009130	0.009130	0.009130	0.00000
10 547169	<-0.00059	<-0.00039	<-0.00092	<-0.00056	<-0.00038	<-0.00038	<-0.00038	0.00000
11 AQC YOWOH	0.009590	0.009567	0.009321	0.009114	0.009234	0.009234	0.009234	0.00000
12 543310	<-0.00059	0.00360	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
13 543338	<-0.00059	0.00067	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
14 543381	<-0.00059	0.00086	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
15 543495	0.00150	0.00550	0.00230	0.00081	0.00120	0.00120	0.00120	0.01261
16 543502	0.00140	0.00350	0.00120	<-0.00063	0.00120	0.00120	0.00120	0.01490
17 543564	0.00210	0.01500	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
18 551271	0.00060	0.00150	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00042
19 543623	0.00170	0.01400	0.01500	0.00530	0.01100	0.01000	0.01000	0.04030
20 543802	<-0.00059	0.01500	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
21 543915	0.00450	0.02000	0.00110	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00110
22 543923	0.00110	0.01300	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
23 543987	<-0.00059	0.00095	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
24 544105	<-0.00059	0.00780	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
25 544233	0.00097	0.00980	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
26 544234	0.00210	0.00560	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
27 544502	<-0.00059	0.00280	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
28 AQC YOWOH	0.009241	0.009517	0.009492	0.009217	0.009211	0.009211	0.009211	0.00000
29 553651	<-0.00059	0.00077	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00039
30 553652	<-0.00059	0.00078	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00039
31 553653	0.00064	0.00072	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00047
32 553654	0.00063	0.00073	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00043
33 553655	0.00060	0.00078	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00042
34 AQC YOWOH	0.009477	0.009143	0.009253	0.009149	0.009270	0.009270	0.009270	0.00000
35 553656	<-0.00059	0.00073	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00041
36 553657	<-0.00059	0.00089	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00040
37 553658	<-0.00059	0.00100	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
38 553659	<-0.00059	0.00064	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000
39 553983	<-0.00059	0.00069	<-0.00092	<-0.00063	<-0.00039	<-0.00039	<-0.00038	0.00000

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 dialog. Links for LIMS can be launched directly from the script on the instrument workstation or can be run at a separate PC workstation in the laboratory.

Figure 4: AqcTools software charting PAH AQC results.



Sample	Name	Data File	Type	Dil.	RT	Final Conc.	Accuracy									
Blank001	Blank - 1-r001.d	Sample	23/04/2010 18:41	1.0	1.318	181.0032		1.753	19.4196		1.413	50.1541		1.561	897.4928	
Blank1	Blank - 1-r001.d	Sample	23/04/2010 18:41	1.0	1.318	181.0032		1.753	19.4196		1.413	50.1541		1.561	897.4928	
Blank1	Blank - 1-r002.d	Sample	23/04/2010 18:44	1.0	0.799	98.3359		1.404	4.9133		1.282	4.9757		1.589	830.6565	
Blank1	Blank - 1-r003.d	Sample	23/04/2010 18:47	1.0	0.801	28.5078		1.841	22.7092		1.418	37.1599		1.739	1.0638	
Blank1	Blank - 1-r004.d	Sample	23/04/2010 18:50	1.0	0.818	66.9247		1.574	17.2583		1.390	35.5841				
Blank1	Blank - 1-r005.d	Sample	23/04/2010 18:53	1.0	0.959	50.6966		1.754	7.1197		1.187	7.9409		1.944	18951.3506	
Extracted1	Cal - 1-r001.d	Blank	23/04/2010 18:56	1.0	1.600	0.0000		1.856	0.0620		1.479	0.0139		1.553	3.4270	
Extracted1	Cal - 1-r002.d	Blank	23/04/2010 19:00	1.0	1.464	0.0000		1.505	0.1284		1.611	0.0000		1.543	3.1553	
Extracted1	Cal - 1-r003.d	Blank	23/04/2010 19:03	1.0	0.773	0.0000		1.442	0.3026		1.183	0.0000		1.539	3.2142	
Extracted7	Cal - 7-r001.d	Cal	23/04/2010 20:18	1.0	1.338	0.5785	94.8	1.392	0.6637	96.2	1.406	0.5169	86.2	1.543	12.5487	103.3

Figure 3: Script used to extract and launch Links for LIMS.

Results Reporting

Rather than introduce further electronic transcription, through for example 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, formatting, handling weights and dilution factors, as well as calculations through to holding of all the necessary data required to upload to LIMS directly. Here's an example (Figure 2) above of instrument results being reviewed. Links for LIMS calculations can be configured to automatically handle duplicate runs. Double clicking an AQC allows historical AQC's to be viewed directly including all limit and trend exceptions. See Figure 4.

Summary

Links for LIMS can fully complement MassHunter extending its utility as well as meeting the requirements for improved AQC responsiveness. Eliminating data transcription from instrument setup and results transfer saves between 3% & 5% errors compared to manual processes, and can save many man hours of effort per run in the immediate post processing of results to allow analysts to react immediately to AQC exceptions.

Further Information

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