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

CSols laboratory systems integration

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Links 4 LIMS

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.

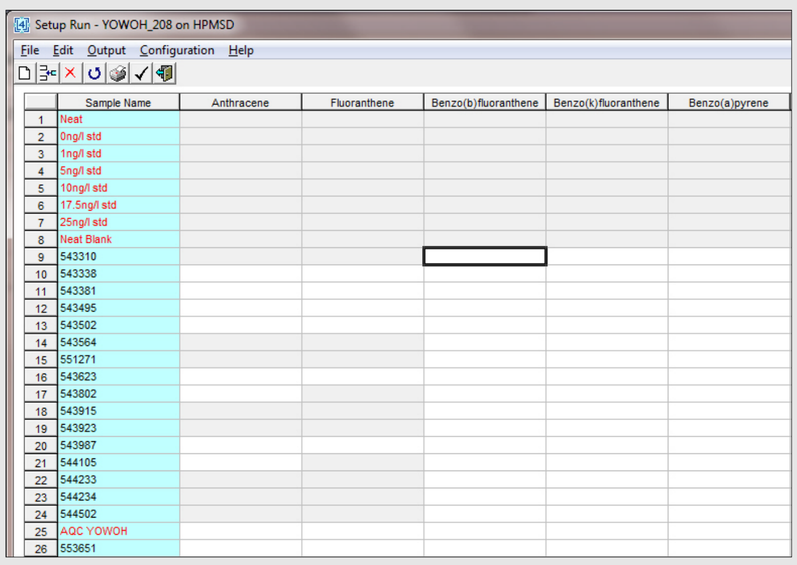

Figure 1: Links for LIMS instrument setup

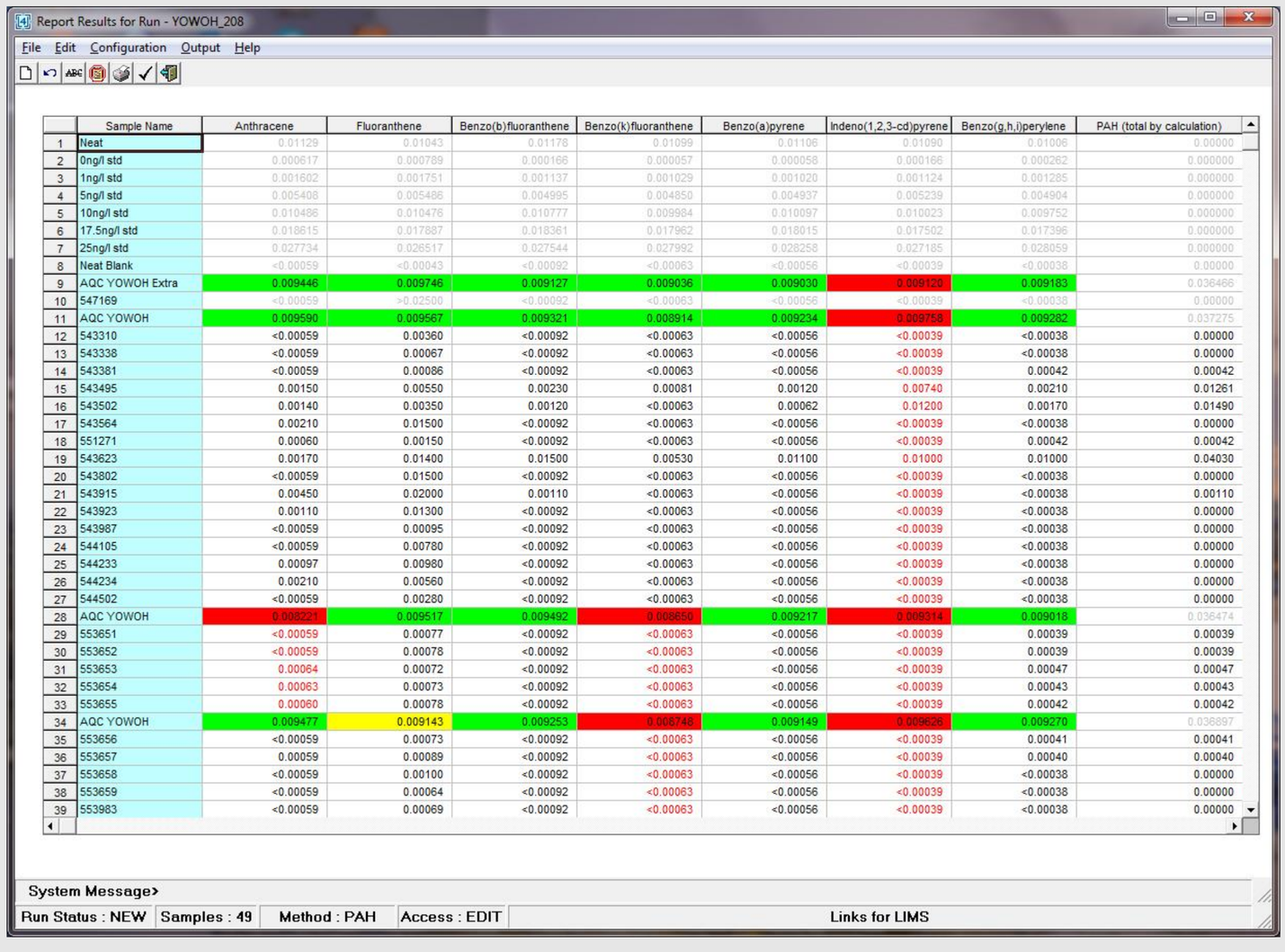

Figure 2: Reviewing results in Links for LIMS

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.

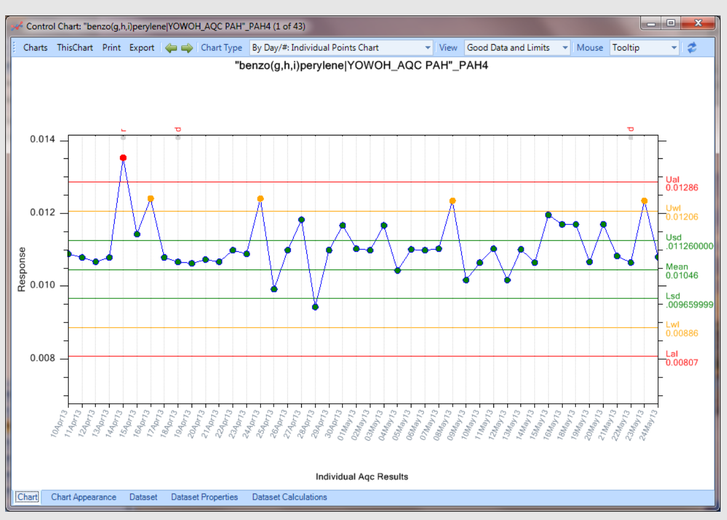

Figure 4: AqcTools software charting PAH AQC results.

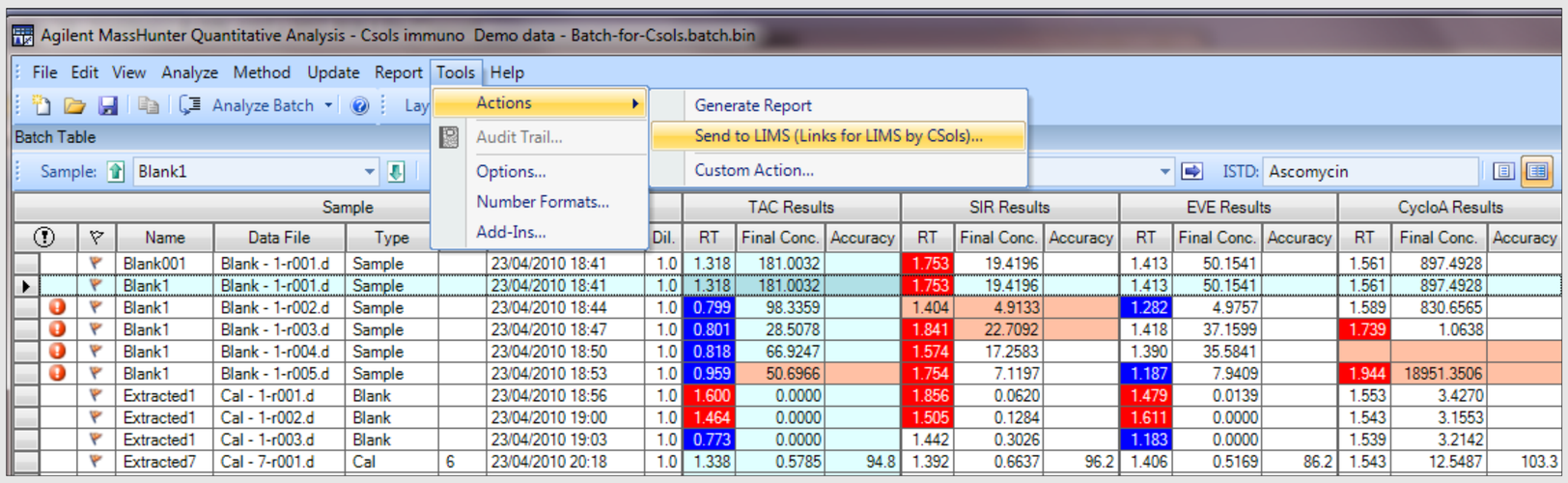

Figure 3: Script used to extract and launch Links for LIMS.

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 AQCs 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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