

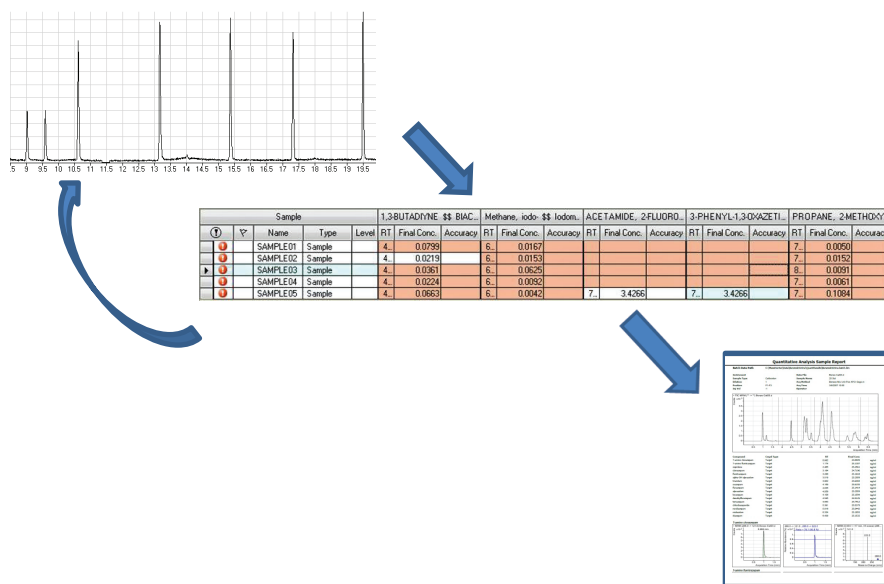
Setting up Post-Run Quantitation and Reporting with MassHunter GC/MS Acquisition Software

Technical Overview

Introduction

Automated quantitation of GC/MS results is an important part of most analytical labs. It is particularly important for laboratories that require immediate analytical results in a high throughput environment, including drug-testing, petroleum, environmental, and food safety laboratories. In addition to routine analysis benefits, post-run quantitation facilitates automated outlier analysis, sample decisions (such as re-injection), and calibration updates. Rapid access to quantitation results enables adjustment of experimental conditions to maximize the utility of the analytical run. The ability to automate post-run quantitation and reporting is therefore absolutely essential to assuring maximum laboratory efficiency.

This technical overview illustrates the ability of MassHunter GC/MS Acquisition software to provide automated data acquisition, quantitation, and reporting. The process is intuitive, fast, and easy to follow, boosting laboratory productivity with just a few clicks of the mouse.



A schematic view of the automated quantitation and reporting process, including its ability to provide rapid feedback to the analytical process.

Setting up an Analytical Sequence to Trigger Post-Run Quantitation and Reporting

Triggering post-run quantitation as part of data acquisition is a simple matter. The post-run quantitation and reporting are defined in the Sequence Table as part of the usual sequence setup. First, configure the Sequence Table to display the **DA Method File**, **DA Method Path**, and **DA Report Template** columns. Note that, as with other sequence information, the settings specified in the columns are used even if the columns are not visible during sequence setup.

To activate post-run quantitation, specify the name of an existing MassHunter Quantitative Analysis (Quant) method in the **DA Method File** field of the Sequence Table (red circle, Figure 1).

Use the **Browse** button at the right-hand side of the **DA Method File** field (arrow in Figure 1) to select the Quant method file, that is, amp.quantmethod.xml, from the saved location. The location is determined when the method is saved within the Quant application. Using the **Browse** button will also populate the **DA Method Path** field to specify the location of the method file. By default, all samples should use the same Quant method and path.

To use a different Quant method, access the **Data Path** column in the Sequence Table to ensure that all collected data is saved to a different folder. If a different Quant method is used with the same data path, samples from the first batch are also included in the second and all subsequent batches.

Running the Sequence

Use the normal **Run Sequence** menu or icon to acquire and process the collected data. All data will be placed in the folder indicated in the **Data File Directory** field (red circle, Figure 2). For those samples with a Quant method defined, a Quantitative Analysis Batch (batch) will be automatically created in the same folder as the data. The batch name will be the acquisition date and Quant method name. Using the example sequence and method shown in Figures 1 and 2, the batch will be named “2011 Sep 06 2044 amp.batch.bin” and will be located in C:\MassHunter\GCMS\1\data\dq1\QuantResults\.

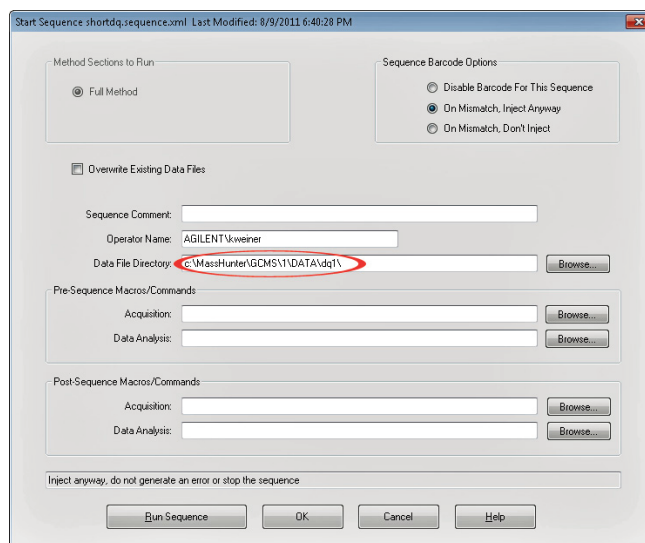


Figure 2. Dialog box from the **Run Sequence** menu, with the designated folder for the quantitation data entered in the **Data File Directory** box (red circle).

| Name | Vial | Method File | Data File | Type | DA Method File | DA Method Path |
|---------------------|------|-------------|-----------|--------|---------------------|------------------|
| 1 Cutoff Calibrator | 1 | cafe1.M | run001 | Cal | amp.quantmethod.xml | C:\MassHunter\DQ |
| 2 Method Blank | 2 | cafe1.M | run002 | Blank | amp.quantmethod.xml | C:\MassHunter\DQ |
| 3 Sample 1 | 3 | cafe1.M | run003 | Sample | amp.quantmethod.xml | C:\MassHunter\DQ |
| 4 Sample 2 | 4 | cafe1.M | run004 | Sample | amp.quantmethod.xml | C:\MassHunter\DQ |
| 5 Sample 3 | 5 | cafe1.M | run005 | Sample | amp.quantmethod.xml | C:\MassHunter\DQ |

Figure 1. The Sequence Table, illustrating the location for the DA Method to be used (in this case a Quant Method), as well as the location of the **Browse** button (arrow) to select the Quant Method file. Note that the DA Report Template column is not shown in this example.

Setting up for Post-Run Reporting

When the sequence has been completed, the newly created batch will contain all the samples, fully processed and ready for final review and reprocessing as necessary in MassHunter Quantitative Analysis (Figure 3).

Specifying post-quantitation reporting is done through the Sequence Table, similar to setting up post-run quantitation. After setting up post-run quantitation, the **Report Template** is specified in the Sequence Table, as shown in Figure 4 (circled)

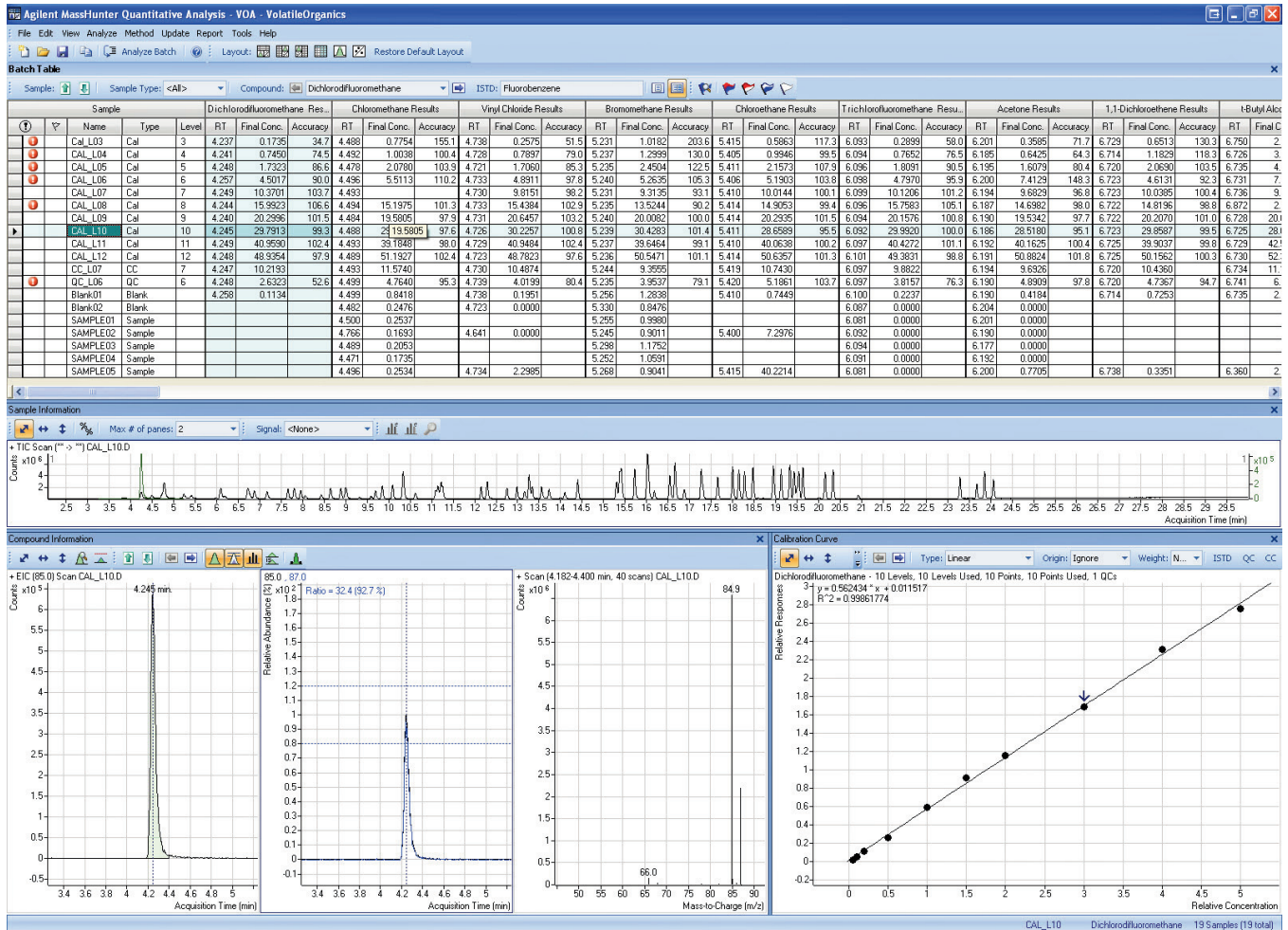


Figure 3. Results of a quantitation sequence run.

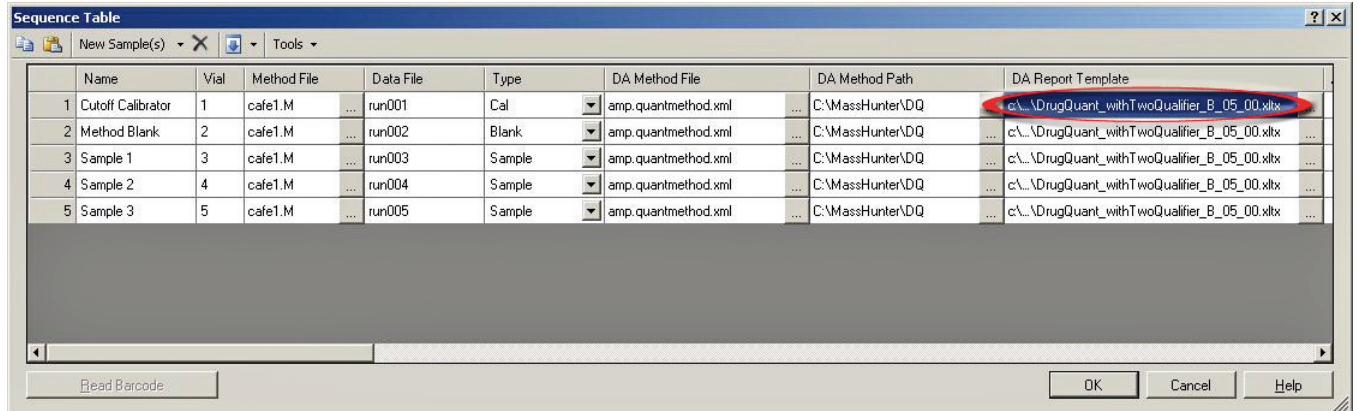


Figure 4. Setting up post-run reporting in the Sequence Table. The name of a valid report template is entered in the DA Report Template box (circled entry).

box). The **Browse** button at the right-hand side of the **DA Report Template** column is used to quickly add the entire path and file name. When the sequence is run, report generation is scheduled on a per-sample basis after quantitation of that analysis has completed.

File Listing from Sequenced Acquisition and Post-Run Quant and Report

The data path specified in the **Data Method Path** column of the **Start Sequence** panel (Figure 2, Data File Directory entry) determines where all data files, batch, quantitation data, results, and reports are saved. The different files and folders created by MassHunter as part of the automatic quantitation and reporting process are shown in Figure 5 (box).

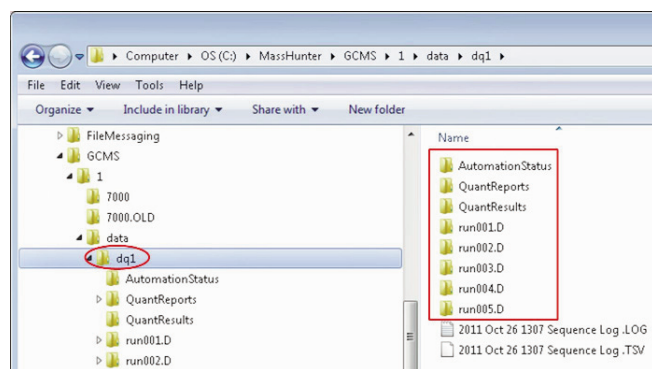


Figure 5. The location of all of the files generated by the automation sequence.

Conclusions

MassHunter for GC/MS analysis provides the ability to automate both quantitation and reporting with just a few clicks of the mouse. Single sample post-run quantitation and reporting is easy to set up in MassHunter GC/MS Acquisition software through the Sequence Table and can provide data acquisition, quantitation, and reporting automation, an essential aspect for all high throughput laboratories. Detailed descriptions of other uses of automated quantitation and reporting for outlier analysis, sample decisions (such as re-injection), and calibration updates will be provided in other technical literature.

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