STREAMLINE LC-MS/MS DATA PROCESSING FOR FOOD ANALYSIS WITH MS QUAN

Jinchuan Yang, Paul Rainville
Waters Corporation, 34 Maple St, Milford, MA 01757; Contact: Jinchuan_yang@waters.com

INTRODUCTION

- The waters_connect™ for quantitation software is a platform that comprises a suite of applications for MS based analyses.
- MS Quan is an application within waters_connect for quantitation platform designed to streamline the LC-MS/MS data processing and review with innovative workflows, data visualization and data navigation tools.
- The overarching key features include batch-level review, task-oriented workflow, and exception-focused individual data review. These key features of the MS Quan application are highlighted here.

EXPERIMENTAL

Samples and Data process:

B vitamins in energy drinks and vitamin B complex dietary supplement were analyzed. The multi-B vitamin analysis was carried out on an Arc™ Premier System coupled with Xevo™ TQ-S micro Mass Spectrometer with MassLynx™ 4.2 for instrument control and data collection.

The LC-MS/MS data sets were processed by the MS Quan Application in waters_connect for quantitation software platform. Details of the B vitamin determination can be found in application note 720007264en.

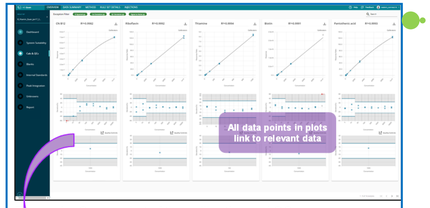

Figure 4a. Screen shot of the calibration and QC page.

Figure 4b. Individual calibration and QC page navigated from the overview page (Fig. 4a).

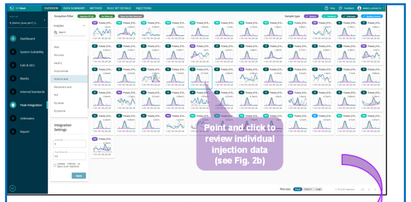

Figure 3a. Screen shot of the Peak Integration overview page

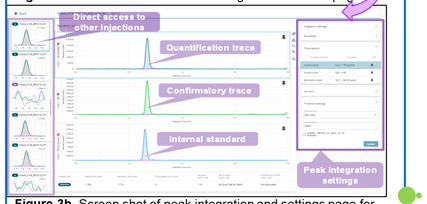

Figure 3b. Screen shot of peak integration and settings page for an individual injection navigated from the overview page (Fig 3a).

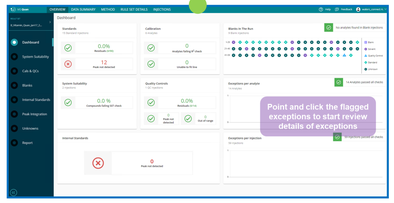

Figure 2. *Screen shot of the Dashboard Results overview. This Dashboard page shows the overall processed results with flagged exceptions. Individual data can be accessed by clicking on each section on this overview page.*

MS QUAN KEY FEATURES

- The complicated LC-MS/MS data processing and review is decoupled into several simple tasks.
- These tasks are carried out in different **task-oriented workflows** in which the user interfaces are tailor designed for the specific workflows. All relevant data and processing parameters, including chromatograms, peak results, method settings, and sample info are placed on the same interface for ease of processing and review.
- The tedious and time-consuming injection-by-injection evaluation process is replaced by a fast **batch-level review** followed by review of individual injection data with additional attention to the exceptions (**Exception-focused individual data review**).
- In the batch-level review, the results from the whole batch are placed side-by-side on the same page, which also allows analysts to easily identify any mistake or error in the processed data (such as improperly integrated peaks) and thus ensure high quality of the analysis.
- These features combined can significantly accelerate the evaluation of the processed data and at the same time improve the overall quality of the analysis.

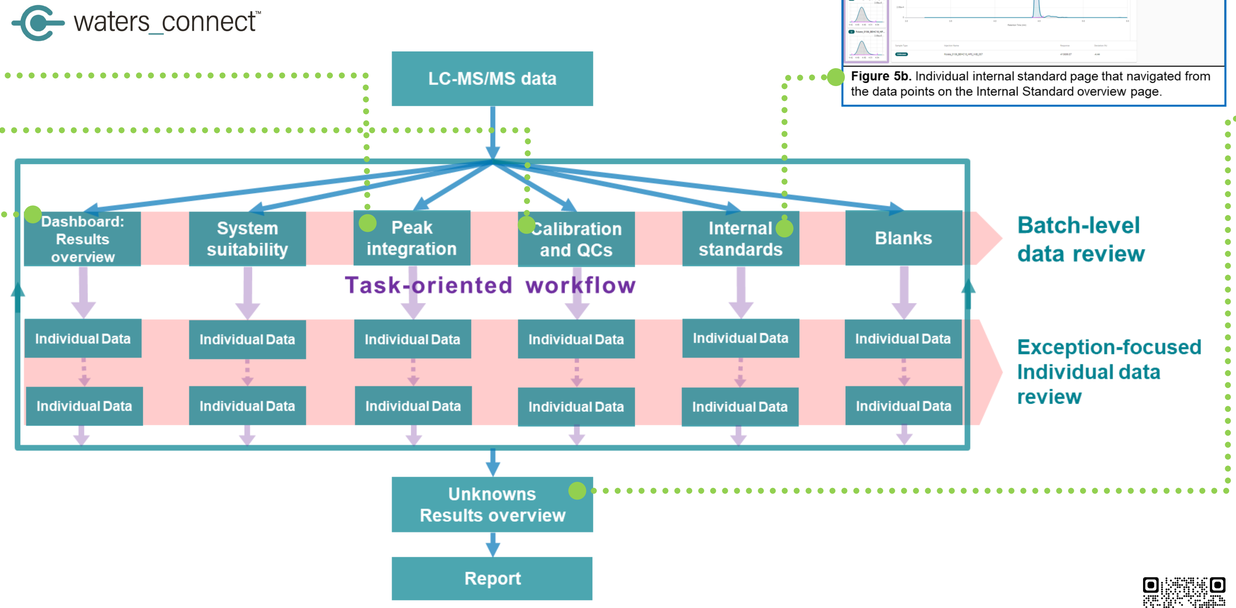

Figure 1. The schematic of main workflows and key features of LC-MS/MS data processing in MS Quan.

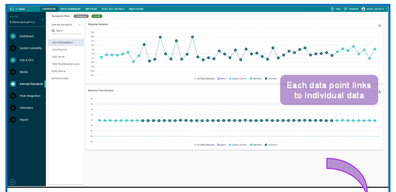

Figure 5a. Screen shot of the Internal Standards page

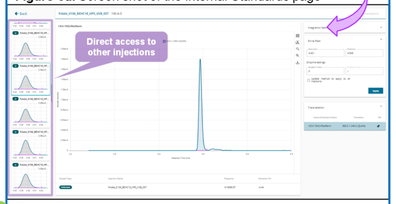

Figure 5b. Individual internal standard page that navigated from the data points on the Internal Standard overview page.

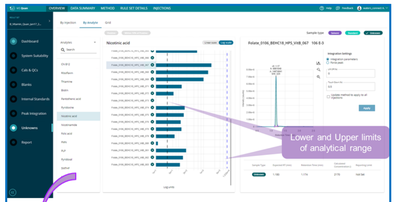

Figure 6a. Screen shot of the Unknows overview page. The Lower and Upper limits of the analytical range are indicated by the dashed vertical lines for each results.

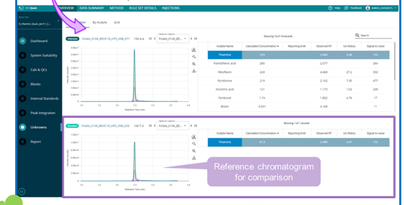

Figure 6b. Individual calibration and QC page navigated from the Unknows overview page (Fig. 6a).

CONCLUSION

- **The MS Quan splits the LC-MS/MS data processing and review into several simpler tasks that are more efficiently carried out by analysts.**
- **Each task starts with an efficient batch-level review followed by more focused individual data processing and review.**
- **The batch-level review improves the consistency in data processing, which reduces errors caused by improperly processed data.**
- **The LC-MS/MS data processing and review is also significantly accelerated by the task-oriented workflow through interactive links and the easy access to all relevant data and settings.**
- **Exceptions are flagged out in MS Quan to facilitate an exception-focused review if desired.**
- **These features in MS Quan allow analysts to efficiently process and review large volumes of LC-MS/MS data and at the same time ensure a high quality of analysis.**

TO DOWNLOAD A COPY OF THIS POSTER, VISIT WWW.WATERS.COM/POSTERS