

LC-MS/MS SOFTWARE DATA PROCESSING AND REVIEW WORKFLOW IMPROVEMENTS FOR CLINICAL RESEARCH

Gareth Hammond¹, Lisa J Calton¹, Christopher Johnstone¹ and Curt Paulette²

¹Waters Corporation, Wilmslow, Cheshire, UK. ²Waters Corporation, 34 Maple Street, Milford MA, 01757 USA

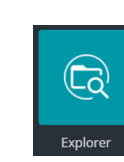
INTRODUCTION

In the field of quantitative LC-MS/MS, the need for efficient, accurate and user-friendly data review software is paramount, with the data generated in the clinical laboratory meeting local guidelines, as well as rigorous method performance characteristics defined by the FDA Bioanalytical Method Validation and CLSI C62-Ed2 guidelines.

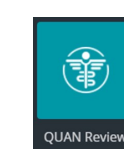
The waters_connect™ for IVD processing software significantly reduces the burdensome aspects of batch quality control by introducing a series of innovative features. These include improvements in workflow, a modernized interface, and the ability to flag exceptions based on rule sets.

WATERS_CONNECT HUB

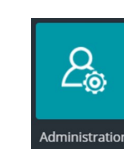
The waters_connect for IVD system consists of a Hub home page from which the following applications can be accessed:



The Explorer application allows you to import MassLynx™ IVD-acquired data into waters_connect for IVD to create a sample set that the QUAN Review application can process.



The QUAN Review application allows you to create processing methods, create rule sets to enable review by exception workflows for data review and review processed data.



The Administration application allows you to create and modify user accounts and their permissions as well as manage the database, system licenses, and global policies.

METHODS

Samples for three multiplexed LC-MS/MS panels with previously defined analytical method performance characteristics were acquired using Waters™ IVD Systems controlled by MassLynx IVD Software. The data was processed, quantified, and reviewed using both the existing TargetLynx™ IVD Application Manager and the new QUAN Review software.

RESULTS

The analytical performance data generated using the new Data Review software compared to the TargetLynx IVD data met the same method performance criteria of the analytical laboratory. For example, a summary of the immunosuppressants precision is given in Table 1.

	QUAN Review		TargetLynx IVD	
	Repeatability (%CV)	Total Precision (%CV)	Repeatability (%CV)	Total Precision (%CV)
Cyclosporine	2.2%	5.9%	2.2%	5.9%
Everolimus	7.8%	7.8%	7.9%	7.9%
Sirolimus	10.4%	11.3%	10.3%	10.8%
Tacrolimus	5.2%	8.0%	5.2%	8.0%

Table 1. Immunosuppressant repeatability and total precision calculated using QUAN Review and TargetLynx IVD.

The mean % bias of External Quality Assurance Sample (n=40) for each analyte processed using Data Review were cyclosporine 7.94%, everolimus -4.15%, sirolimus -0.97% and tacrolimus 4.59% respectively whilst the mean % bias calculated using TargetLynx IVD were cyclosporine 7.94%, everolimus -4.04%, sirolimus -0.70% and tacrolimus 4.35% respectively.

AN OPTIMIZED LC-MS/MS QUANTIFICATION DATA WORKFLOW WITH A REDUCED REVIEW TIME OF UP TO 50%

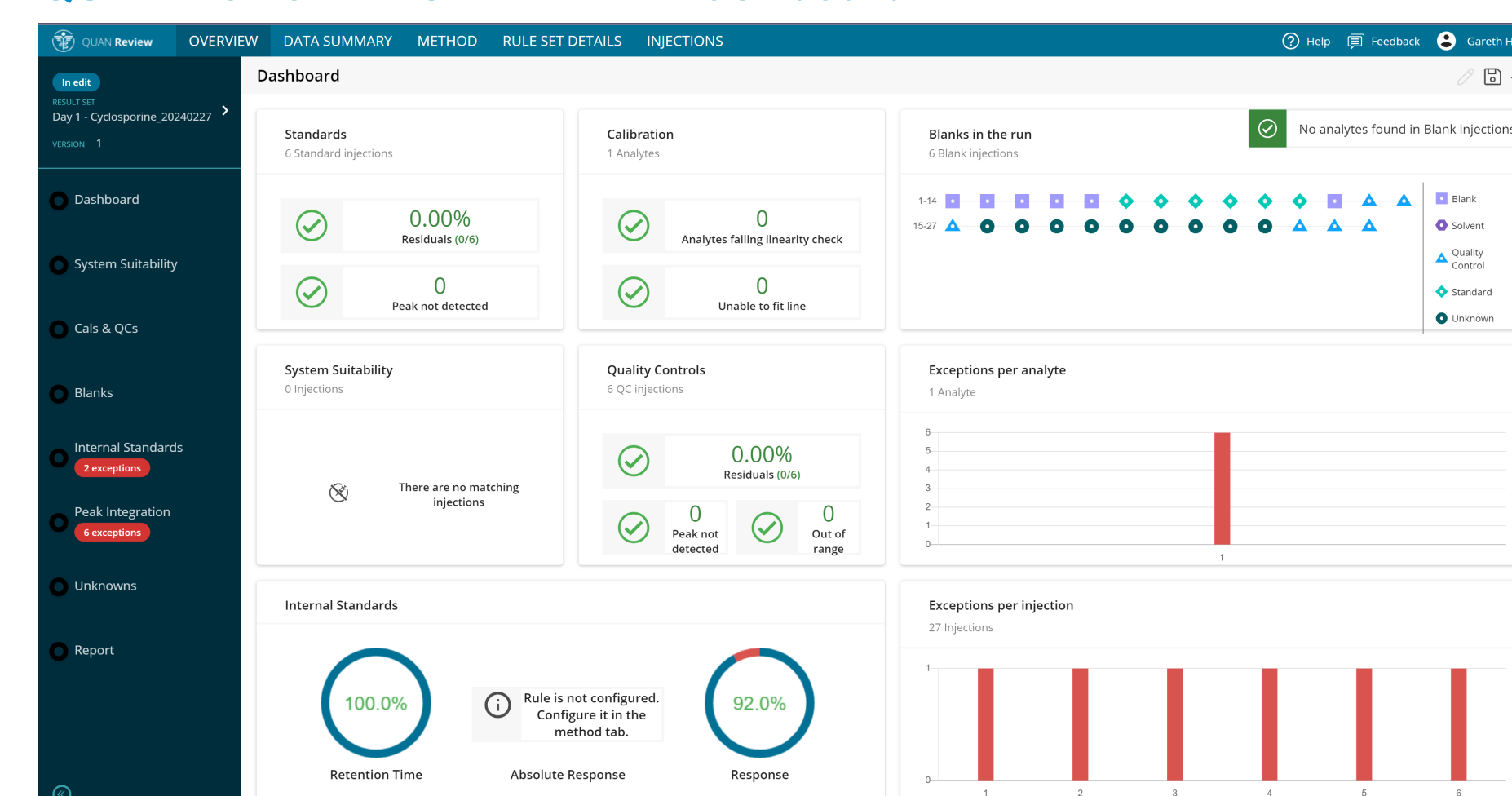
WORKFLOW



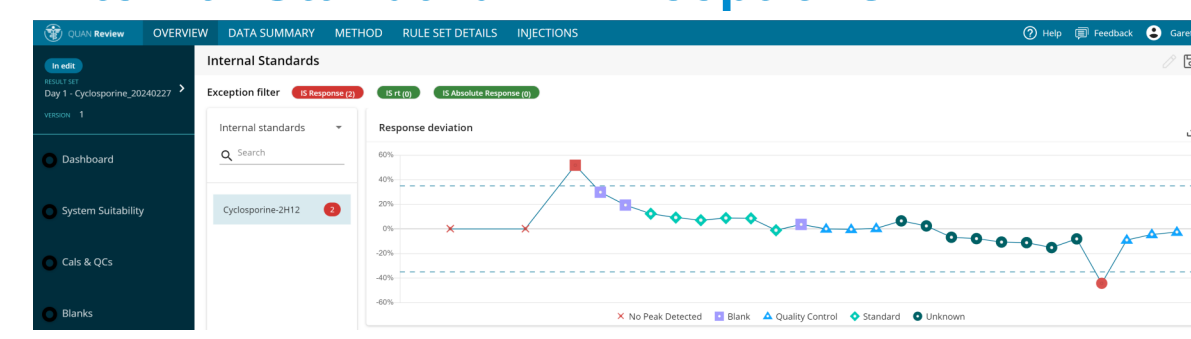
Many benefits of the simple to use software include:

- immediate view as to whether the batch has passed
- focused review by exception using rule sets
- trending internal standard response and retention time
- a user friendly interface
- multiple chromatogram review to quickly identify data quality issues (e.g. peak shape, retention time and interferences)
- batch level review
- simplified task-oriented accelerated workflows decouple complicated data review into several simplified tasks
- reduction in time taken to review large multiplexed panels

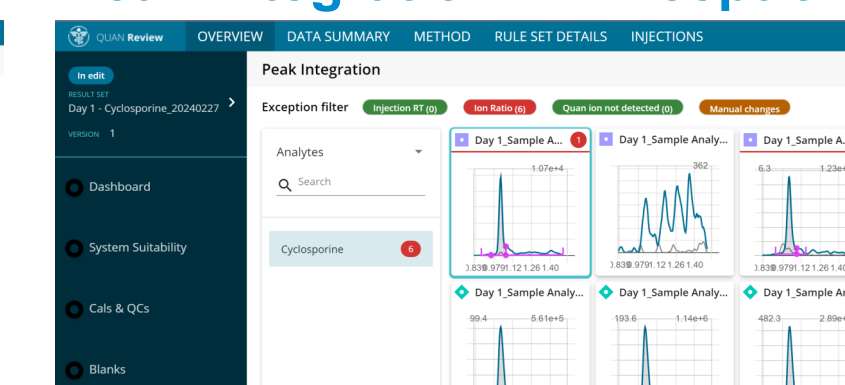
QUAN Review — OVERVIEW Dashboard



Internal Standard — Exceptions



Peak Integration — Exceptions



CONCLUSION

- The exception focused review functionality allowed tailored rule sets which reduced the time spent reviewing data by up to 50%.
- The batch-level review and task-oriented workflow improved batch acceptance and simplified the review of complicated datasets into easy tasks.
- The new QUAN Review Software generated results equivalent to the existing TargetLynx IVD Application Manager.

For Research Use Only. Not for use in diagnostic procedures.

Waters, waters_connect, MassLynx and TargetLynx are trademarks of Waters Technologies Corporation.

©2024 Waters Corporation