STREAMLINED SOFTWARE FOR ROUTINE LC-MS/MS DATA PROCESSING

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INTRODUCTION

LC-MS/MS analyses generate large and complex datasets, making data processing and review time- and expertise-intensive and often the primary bottleneck in analytical workflows. The waters_connect™ for Quantitation platform was developed to address this challenge. This software platform hosts a suite of browser-based applications for efficient chromatographic data management. Among these, MS Quan is specifically designed to streamline LC-MS/MS data processing and review. This study highlights the key features of MS Quan for improving efficiency and quality in data processing and review in LC-MS/MS analysis of free inositol stereoisomers in foods.

OBJECTIVES

The goal of this work is to evaluate MS Quan for LC-MS/MS data processing and review in the analysis of free inositol stereoisomers in foods.

DATA PROCESSING AND REVIEW

Method

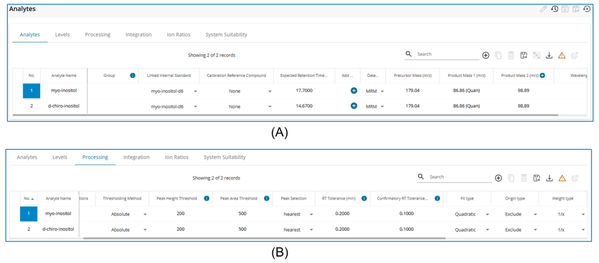

Figure 1. Screenshots of selected method parameter tables. (A) Analytes Table; (B) Processing Table.

Rule Set

Table 1. Rule Set criteria applied to the data processing in LC-MS/MS analysis of free inositols in foods.

	Rules
Calibration and QC	
R Square Value:	$R^2 \geq 0.990$
Calibration Deviation:	Relative residual error ≤20%
Signal to noise ratio:	≥10
Internal Standard	
Internal Standard Response:	≤30% from the median response of IS in the batch
Internal Standard RT:	≤15 sec from the expected RT
Peak Integration	
Injection RT:	≤1% from the mean detected value of the Reference
Ion Raio:	≤30% from the values specified in the Method
Blanks	
Blank response:	≤20% of the area of the Lowest level of calibration standard

Overviews

Dashboard

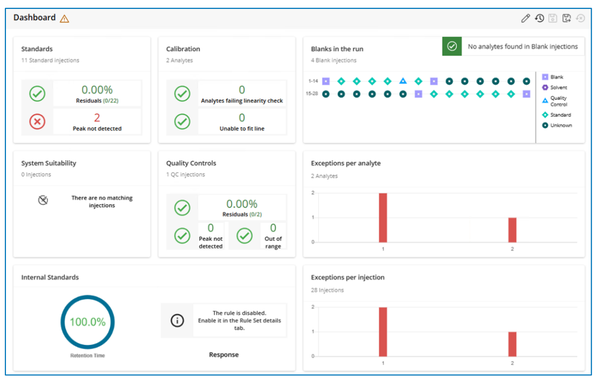

Figure 2. Screenshot of the Dashboard Overview.

Peak Integration

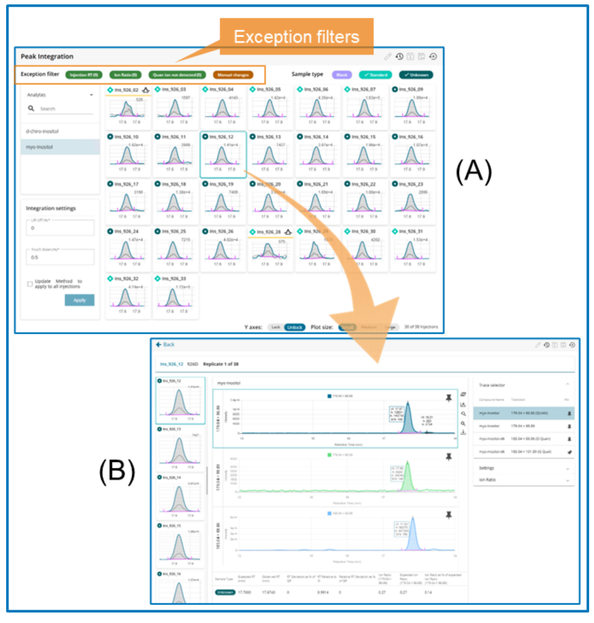

Figure 3. Screenshots of the Peak Integration Overview (A) and the individual injection peak integration review (B), accessible by clicking on the chromatogram image on the Overview page (indicated by the arrow). Exception filters are shown on the Peak Integration Overview page.

Calibration

Figure 4. Screenshots of the Peak Integration Overview (A) and the individual injection peak integration review (B), accessible by clicking on the chromatogram image on the Overview page (indicated by the arrow). Exception filters are shown on the Peak Integration Overview page.

Internal Standards

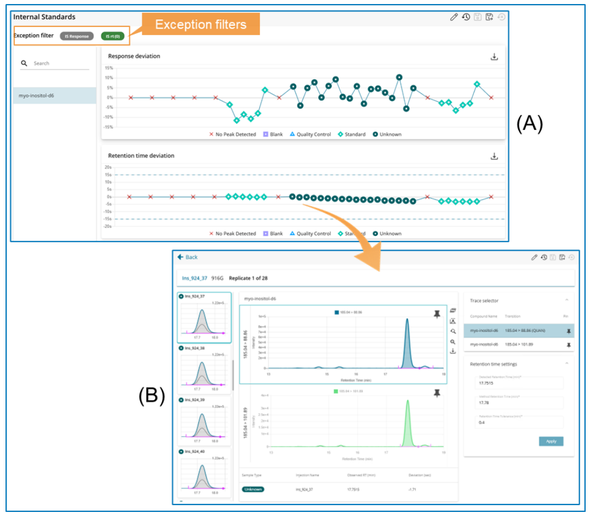

Figure 5. Screenshots of the Calibration Overview (A) and the individual calibration point review (B), accessible by clicking on a data point on the Overview page (indicated by the arrow). Exception filters are also highlighted on the Overview page.

RESULTS AND DISCUSSION

Identical results were obtained for all samples by TargetLynx™ Software and MS Quan.

Table 2. Comparison of results processed in TargetLynx Software and MS Quan.

	Results Processed in TargetLynx				Results Processed in MS Quan			
	myo-Inositol		*D-chiro*-Inositol		*myo*-Inositol		*D-chiro*-Inositol	
	Mean Conc. (mg/100 mL)*	RSD (n=3)	Mean Conc. (mg/100 mL)	RSD (n=3)	Mean Conc. (mg/100 mL)*	RSD (n=3)	Mean Conc. (mg/100 mL)	RSD (n=3)
Soybean milk	4.16	2.98%	3.10	2.34%	4.16	2.98%	3.10	2.34%
Almond milk	2.46	0.63%	N.D.		2.45	0.63%	N.D.	
Oat milk	0.64	7.18%	N.D.		0.64	7.19%	N.D.	
Whole milk	3.13	1.69%	N.D.		3.13	1.69%	N.D.	
Corn meal	34.72	2.15%	N.D.		34.69	2.15%	N.D.	
Infant formula	83.45	1.14%	N.D.		83.44	1.14%	N.D.	

Note: * mg/100 g for corn meal and infant formula.

CONCLUSION

The Overview screens

- Enable rapid, side-by-side comparisons of all injections across the entire batch.
- Allow direct access to chromatograms, results, and processing parameters from a single screen.
- Offer layouts tailored to specific sample types and processing tasks.

Task-oriented workflow

- Task-specific layouts streamline data review and process by eliminating the need to navigate between multiple screens.
- Simplifies workflows and improves efficiency.

The Rule Set criteria

- Automatically flag exceptions and anomalies.
- Support thorough data evaluation while minimizing process error.

MS Quan offers an intuitive, efficient software solution for routine and high-throughput LC-MS/MS analyses.

Reference

1) Yang, J., Harden, S., and Rainville, P. Streamlined LC-MS/MS Data Processing with waters_connec for Quantitation: Application to Free Inositol Analysis in Foods, Application Note 720009238, Waters Corporation, 2026.

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