Improving Routine Quantitation Workflows in SCIEX OS-MQ

Streamline processing and review of quantitation data with new features in SCIEX OS.

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What: Advances in technology have resulted in a need for higher and faster sample throughput, with increasing number of measured analytes per sample. A greater strain on necessary data analysis steps leads to a bottleneck of data processing and review for chromatographic peak integration, quality of calibration curve, and more.

The new SCIEX OS-MQ software brings routine quantitation workflow to the next level for quicker turnaround time. The sleek, intuitive user interface overlies a sophisticated peak integration algorithm, new features to automatically remove outliers from a calibration curve, and new tools for flagging and filtering results. These features combine to make data processing and review more streamlined and efficient. In an example of 193 analytes with 9 calibrator levels acquired in triplicate, the processing took about **1 minute**, compared to 180 minutes to manually review and approve all calibration curves for the same data set.

How: The new **Auto Peak integration** algorithm is designed for **more consistent integrations**, meaning fewer manual integrations. Fewer parameters for the user to set in building the processing method allows for more efficient method optimization and data review.

Automatic Outlier Removal allows the user to set criteria for the automatic removal of standard outliers from the calibration curve. The user controls what regression linearity, accuracy of standards, precision of replicates, and outlier tolerance are acceptable, and the algorithm then **builds the calibration curve for each standard to meet the defined criteria**. The algorithm helps to alleviate the pain of manually establishing many acceptable calibration curves when working with many analytes varying in sensitivity and performance. Both features help to maintain **consistent results among different analysts** working on the same method.

1) Calibration curve with outlier points (hollow) removed by Automatic Outlier Removal to quickly and automatically provide criteria-meeting quantitation and calibration.

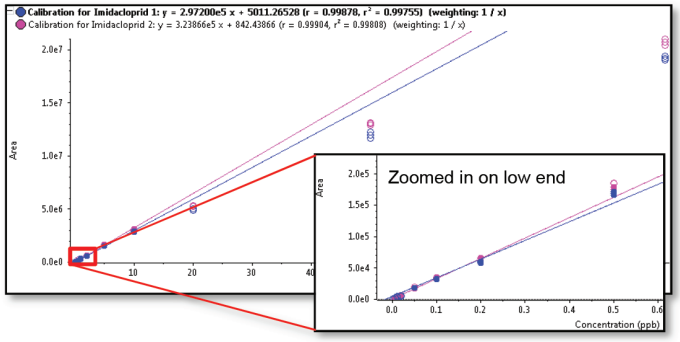
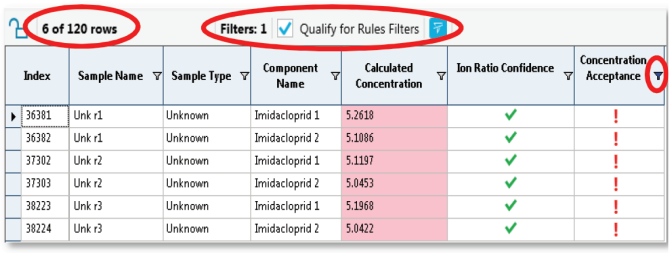


Figure 1. In a method with hundreds of transitions, significant amount of time is taken to review data and adjust each calibration curve. Automatic Outlier Removal simplifies the review by using only standards that meet calibration curve criteria.

2) Unknown samples that fail the Concentration Acceptance criteria are flagged, and then the column can be used to filter out those samples that are above a defined concentration limit for the selected analyte. The table shows how many rows are displayed out of the total number of rows, as well as how many filters are applied to the data set.



Index	Sample Name	Sample Type	Component Name	Calculated Concentration	Ion Ratio Confidence	Concentration Acceptance
36381	Unk r1	Unknown	Imidacloprid 1	5.2618	✓	!
36382	Unk r1	Unknown	Imidacloprid 2	5.1086	✓	!
37302	Unk r2	Unknown	Imidacloprid 1	5.1197	✓	!
37303	Unk r2	Unknown	Imidacloprid 2	5.0453	✓	!
38223	Unk r3	Unknown	Imidacloprid 1	5.1968	✓	!
38224	Unk r3	Unknown	Imidacloprid 2	5.0422	✓	!

Figure 2. The columns in the Results Table each have individual filtering capabilities. Review is simplified by showing only samples that match relevant criteria. This quickly reduces the time to identify positive hits in a large sample batch.

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