

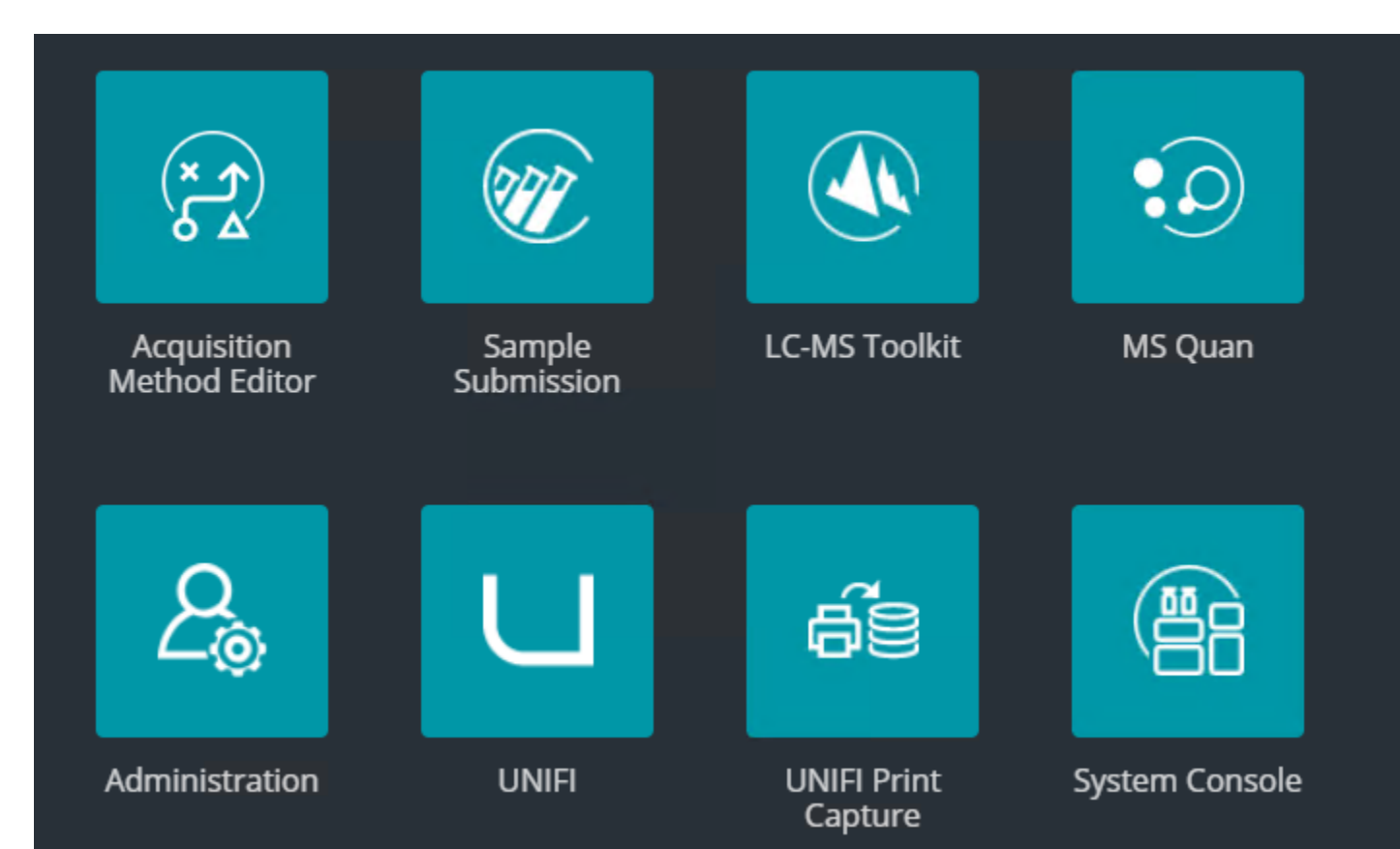
A simple, easy, and efficient way to process and review data for large methods using the MS Quan app within the new waters_connect™ software



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Running a targeted method for quantitation of large numbers of analytes, across many batches of different samples, presents food testing laboratories with several challenges. Issues associated with developing, managing, and curating error-free acquisition and data processing methods and the review of data can be both time-consuming and cumbersome. To help overcome these daily challenges, we are showcasing the new MS Quan app that is included within the new waters_connect software platform. We will demonstrate the usability of the software by generating a processing method from acquired data, efficiently process, and review the quantitative data with a focus on a workflow utilizing exception focused review. We will demonstrate the ease of setting up batch QC criteria such as calibration correlation, residuals, QC check, blanks, internal standard response, ion ratio and retention time tolerances, as per documented guidelines or bespoke values. A batch dashboard immediately gives the user an overview of the health of the batch and highlight potential areas that require user intervention to aid laboratory efficiency. There are many enhancements that allow users to view many chromatograms on one screen at once, totals, isotope dilution, standard addition and many more new features are available now. Come and join us for a glimpse of this new user-friendly software.

Data processing can indeed be a time-consuming task, especially when dealing with large number of analytes and samples. However, with the help of various applications such as Acquisition Method Editor (AME), Sample Submission, LC-MS Toolkit and MS Quan applications, waters_connect software makes data acquisition and processing more efficient and streamlined.



Various applications within waters_connect™ HUB software to perform quantitative analysis.

Waters_connect HUB offers various applications to control and setup instrument systems for LC-MS/MS data acquisition and data processing.

Acquisition Method Editor (AME)

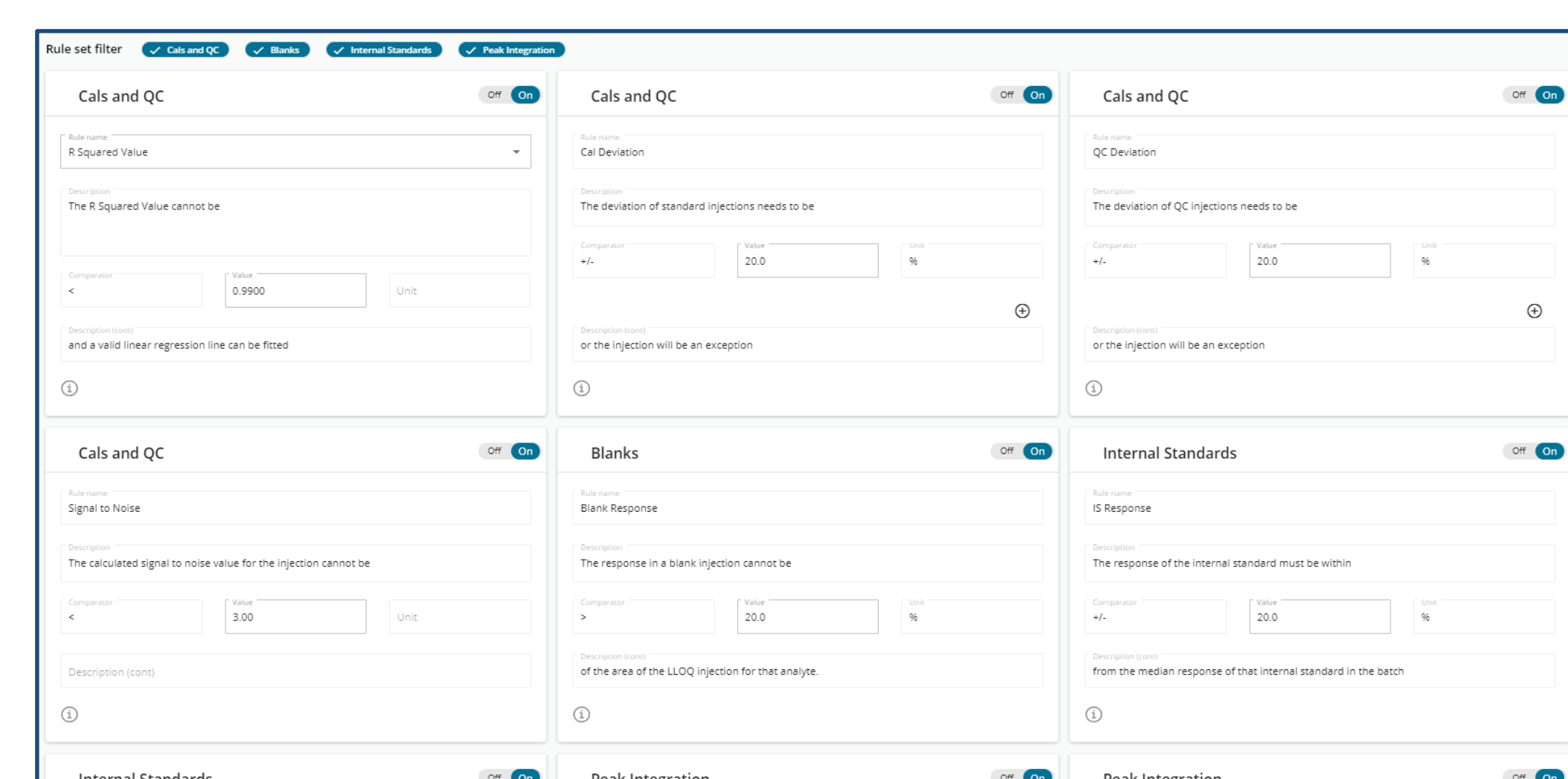
Liquid chromatography and mass spectrometry related parameters are defined in AME. Multiple compounds optimized for MRMs in system console can be transferred error-free into AME to generate the MS method. With a single click users can generate a MS Quan processing method from AME. The error-free and single click reduces time to build cumbersome MS method and processing methods.

Analyte name	% IS	Precursor mass	Product mass	Polarity	Core voltage (V)	Collision energy (eV)	Quan	Retention time (min)	Start time (min)	End time (min)	Soft ionization	Precursor resolution	Product resolution	Auto detect	Dwell time (min)
Abamectin B1a	895.46	327.02	Positive	76	52	13.38	12.88	13.88				UNIT	UNIT		17.0
Abamectin B1a	895.46	791.22	Positive	76	44	13.38	12.88	13.88				UNIT	UNIT		17.0
Acephate	184.00	95.00	Positive	10	25	2.50	2.00	3.00				UNIT	UNIT		5.0
Acephate	184.00	124.90	Positive	10	18	2.50	2.00	3.00				UNIT	UNIT		5.0
Acetamiprid	223.01	56.10	Positive	30	20	3.99	3.49	4.49				UNIT	UNIT		4.0
Acetamiprid	223.01	126.00	Positive	30	20	3.99	3.49	4.49				UNIT	UNIT		4.0
Acibenzolar-s-methyl	210.90	69.00	Positive	25	35	7.28	6.78	7.78				UNIT	UNIT		3.0
Acibenzolar-s-methyl	210.90	135.90	Positive	25	30	7.28	6.78	7.78				UNIT	UNIT		3.0
Aldicarb	213.11	89.10	Positive	35	20	4.54	4.04	5.04				UNIT	UNIT		3.0
Aldicarb	213.11	116.10	Positive	35	11	4.54	4.04	5.04				UNIT	UNIT		3.0

Acquisition Method Editor showing MS method with analyte name, precursor mass, product mass, retention time, retention time window, dwell time etc.

MS Quan Rule Set : Exception Focused Review

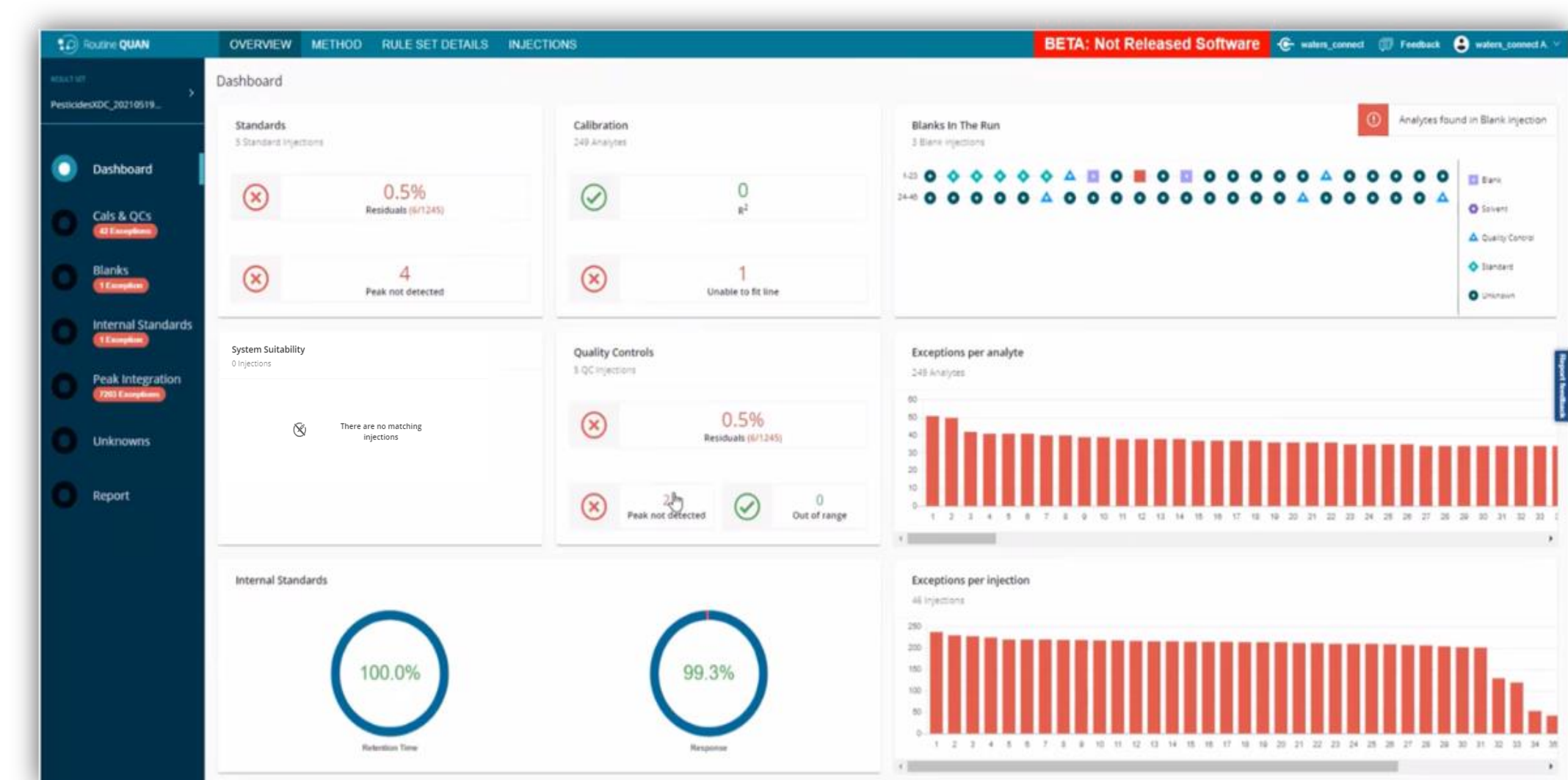
Exception focused review within the software reduces the time it takes for users to review their data by using tailored rule sets and focus the review process on the injections and analytes where user intervention is needed.



Example of rule set for exception focused review: Users can setup acceptance and tolerance criteria for calibration and QC (R and R squared value, deviation, signal to noise ratio, blank response compared to LLOQ injection, internal standard (retention time and response), peak integration (retention time, ion ratio and quantifier ion detected) according to guidelines.

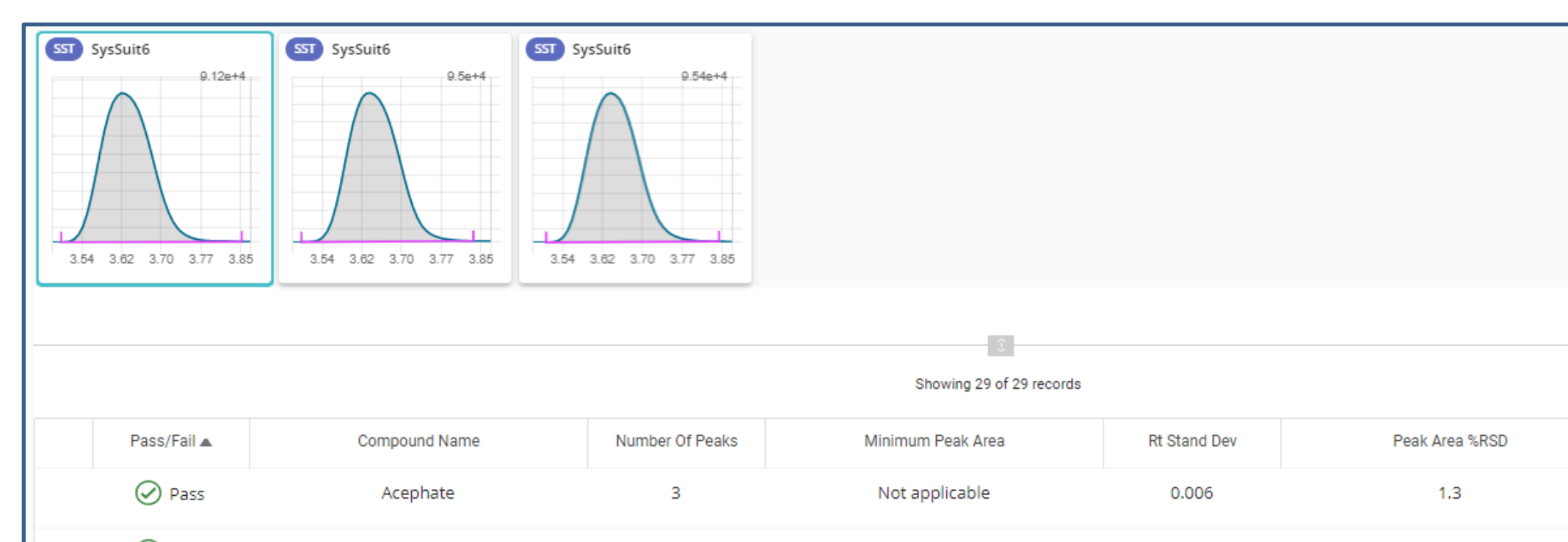
MS Quan : Quantitative workflow

Dashboard : Based on the Exception Focused Review (XFR) criteria, MS Quan will filter results to the injections that have fallen outside the user-determined ruleset. Dashboard provides overall view of the sample batch.



Dashboard displays overall batch results: standards, calibration, QCs, unknown, internal standard, sample batch, exception per analyte and injection.

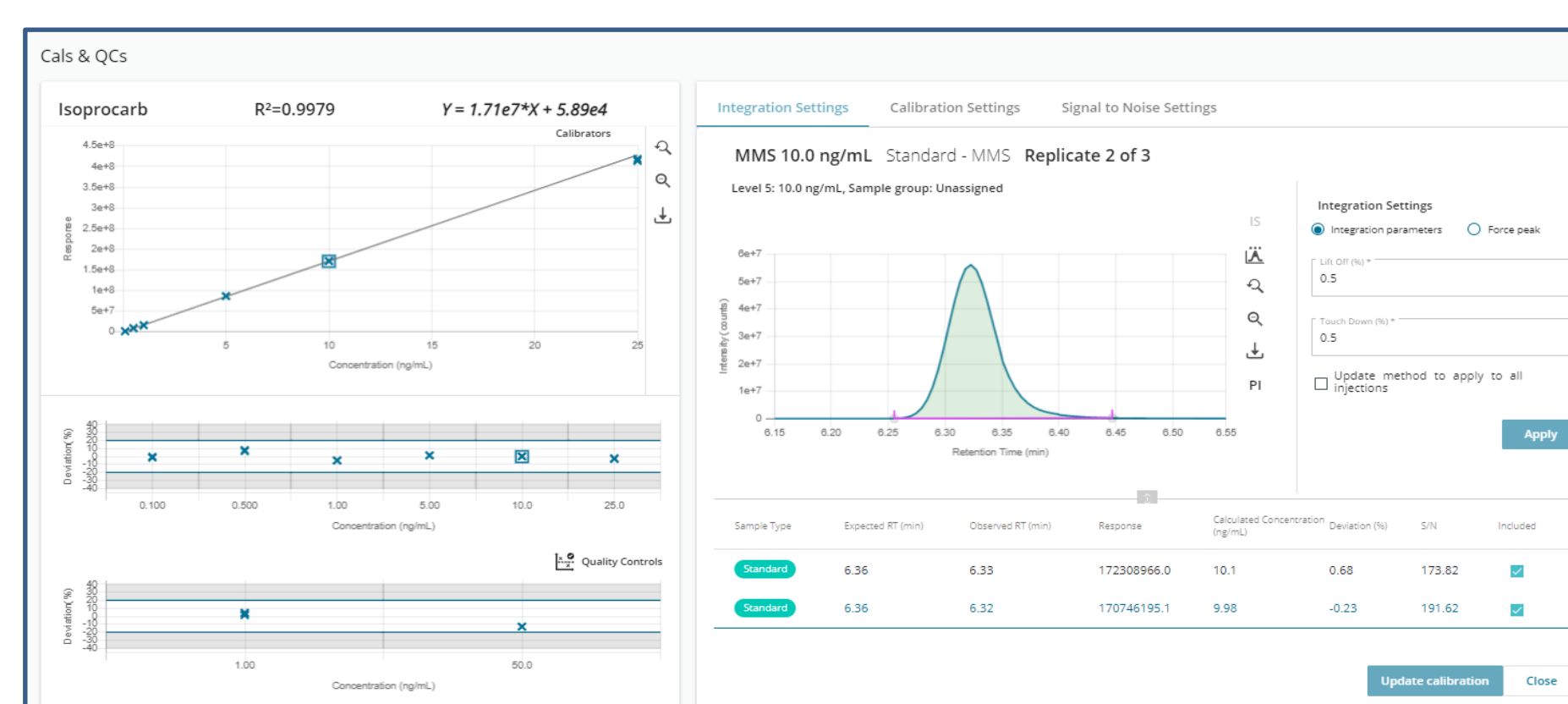
System suitability: User can pre-define criteria in the MS Quan method for system suitability injections. Pass or fail criteria for analytes as well as internal standards can be set on minimum peak area, retention time standard deviation, peak area %RSD and ion ratio.



System suitability injections.

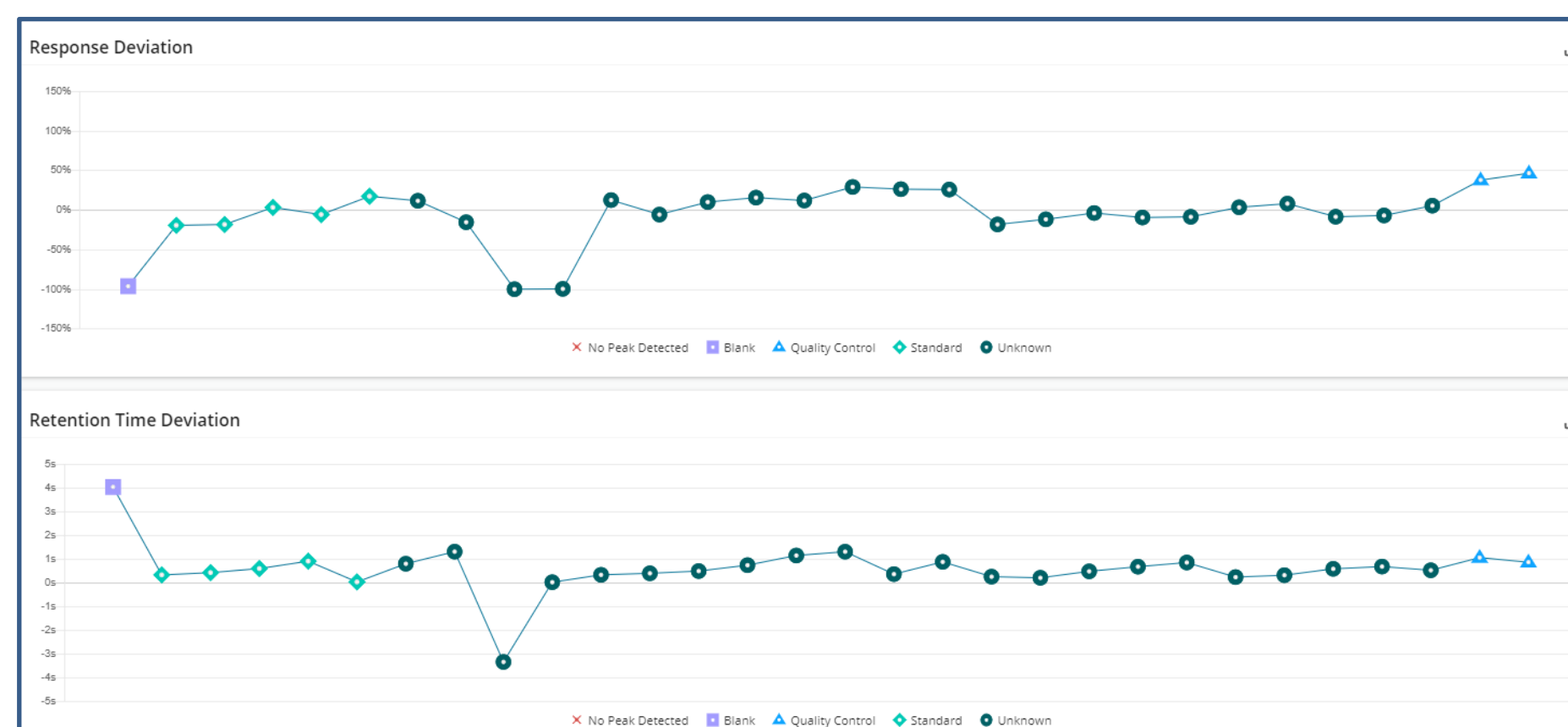
Cals & QCs: Calibration is displayed for all analytes with linearity, deviation, deviation for QCs, chromatograms, expected and observed retention time, calibration & integration settings and signal to noise ratio. The user can make changes to the integrated peaks and update the method to apply for all injections with single click. Any outliers will appear in red as an exception with description of it.

Blank : Any peak observed in sample type "blank" will be shown here. Response of the blank samples gets calculated automatically against LLOQ injection and if it is outside of the criteria set in rule set it will appear as an exception.



Cals & QC for Isoprocarb with R², line equation, chromatogram, retention time, calibration and integration settings and signal to noise.

Internal Standard: Trend plot of internal standard response deviation and retention time deviation across the sample batch.



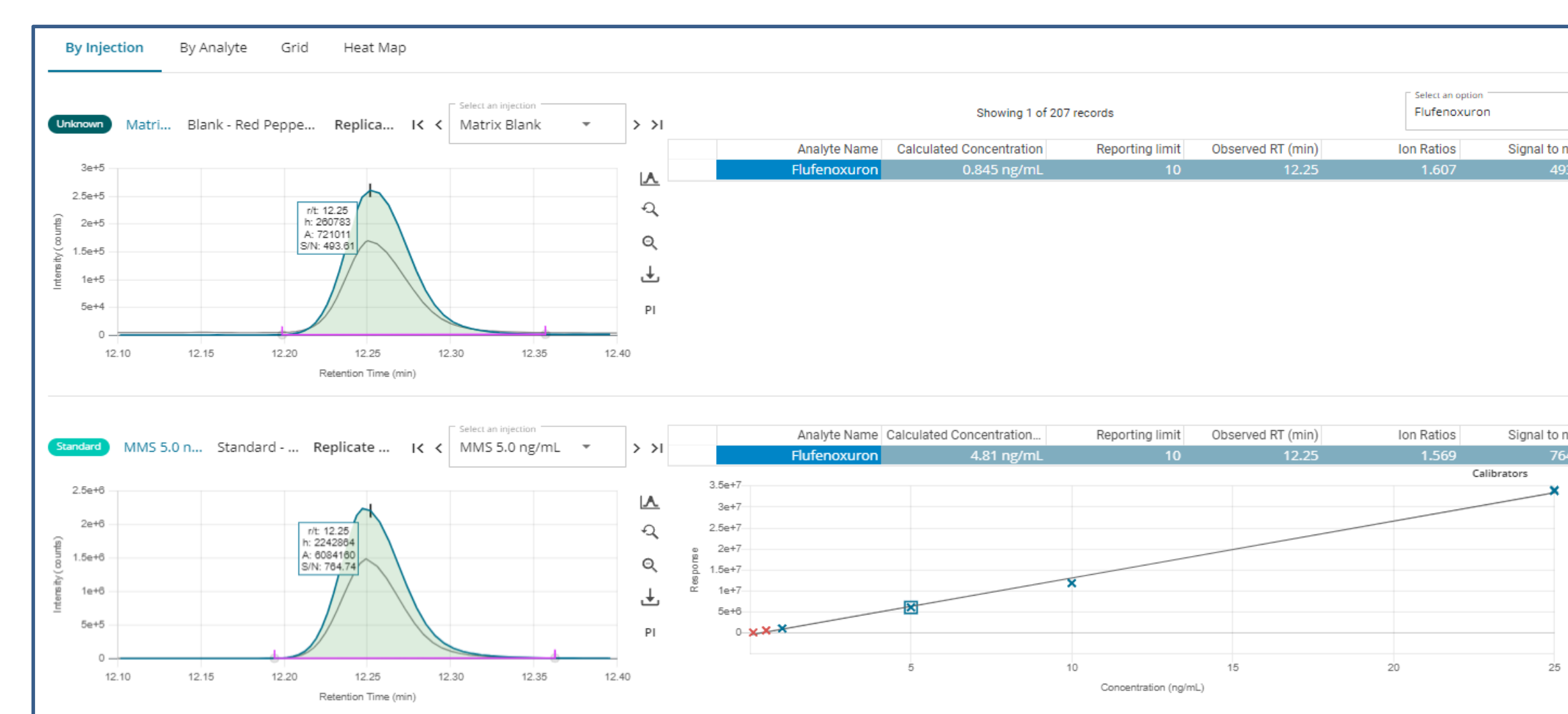
Internal standard plot of response and retention time deviation for blank, quality control, standards and unknowns.

Peak Integration: Overlay of chromatograms showing integrated quantifier and qualifier transitions for all sample types in one place for quick data review. The user can also filter the sample type.



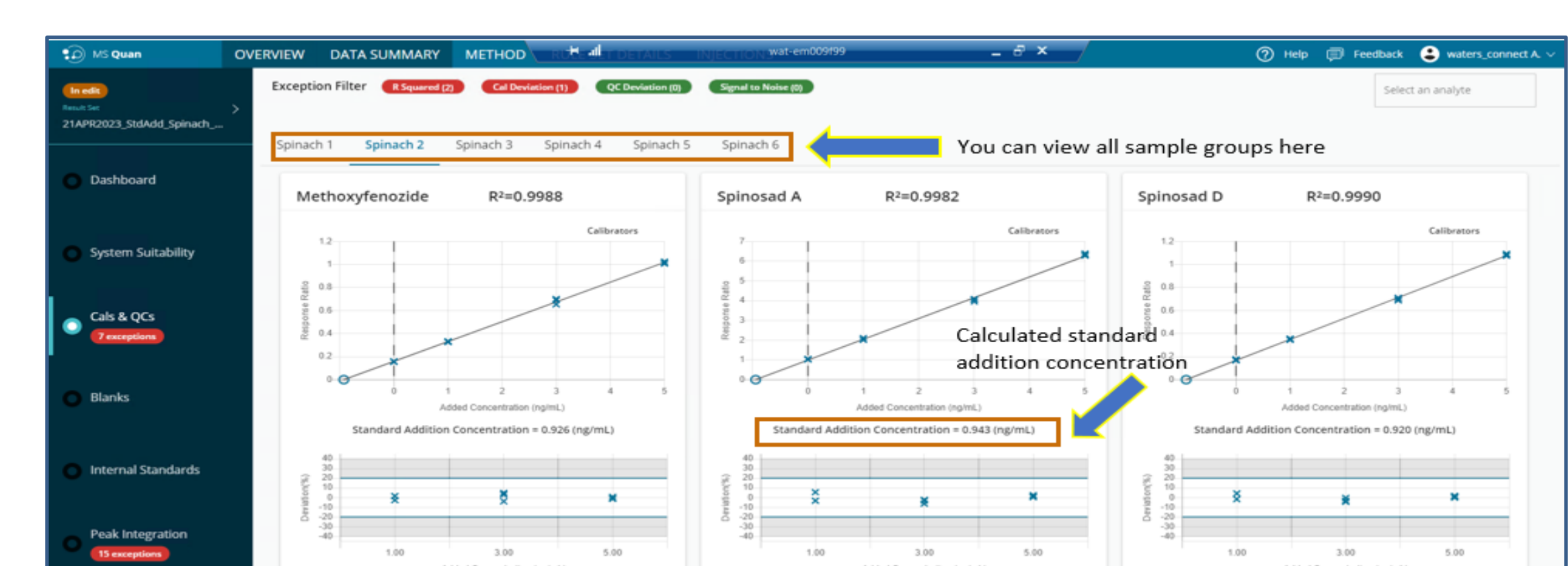
Chromatograms of all sample type in one view.

Unknowns : Users can view chromatograms of unknown (top) and standard (below) simultaneously with calculated concentration of unknown sample, retention time, peak shape, peak area, peak height, signal to noise range and calibration curve. Concentration of unknown samples can be viewed by injections, analyte, grid or by heat map.



Calculated concentration of unknown along with chromatograms of unknown and standard.

Standard Addition: Allows users to quantitate samples using standard addition methodology to deal with samples where blank matrix is not available or matrix interference cannot be overcome. Sample groups can be pre-defined in Sample Submission to allow multiple standard addition results in a single result set.



Multiple standard addition results in a single result set.

Totals, isotope dilution and concentration factors : User can also perform totals, isotope dilution and concentration factors within MS Quan and does not require use of other software.

Don't miss out this great opportunity to know how you can review your data faster with Exception Focused Review. For more information, please visit our website @ videos.waters.com or stop by at Waters booth.

Come and visit Waters booth for live demo of waters_connect software

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CONCLUSIONS

- Waters_connect™ Accelerated workflows that speed up and enhance fast data processing of large sample batches.
- Up to 50% reduction in time spent on data review with the unique Exception Focused Review (XFR) functionality.
- Standard addition, totals, isotope dilution, concentration factors and user-friendly functionalities available in waters_connect software.