

Solving Analytical Challenges in PFAS Testing: Robust Calibration Data, Low Mass Confirmation and Isomer Quantification

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Introduction

Per- and polyfluoroalkyl substances (PFAS) are widely monitored due to their persistence and growing regulatory scrutiny, requiring accurate identification, quantification, and confirmation across diverse environmental matrices. Laboratories must achieve high analytical reliability while maintaining throughput, yet frequent method recalibration remains time-consuming and costly due to expensive standards and complex workflows. In addition to calibration challenges, difficult matrices such as landfill leachate and biosolids introduce matrix effects, while short-chain PFAS like PFBA and PFPeA lack conventional product ions for confirmation. Furthermore, regulatory requirements often demand flexible reporting of branched, linear, and total PFAS isomers.

This study evaluates the robustness and analytical performance of the Xevo™ TQ Absolute XR Mass Spectrometer with waters_connect™ for Quantitation Software. Using extended, high-throughput analysis of surface water, biosolids, and landfill leachate, it assesses calibration longevity, QC stability, and the reliable quantitation and confirmation of challenging PFAS compounds over prolonged operational periods.

Robust Calibration Data

Method calibrations were generated for 42 PFAS analytes using linear, 1/x weighted calibration curves, all of which returned relative standard error (%RSE) values below 20%, demonstrating appropriate calibration quality at the outset of the study. These calibrations were subsequently challenged over extended analytical sequences involving repeated injections of surface water, biosolid, and landfill leachate extracts. Quality control standards were injected every ten matrix samples and evaluated against the original calibration curves using a $\pm 30\%$ tolerance criterion. The Xevo TQ Absolute XR Mass Spectrometer maintained method calibration integrity for up to 5 weeks as shown in Figure 1.

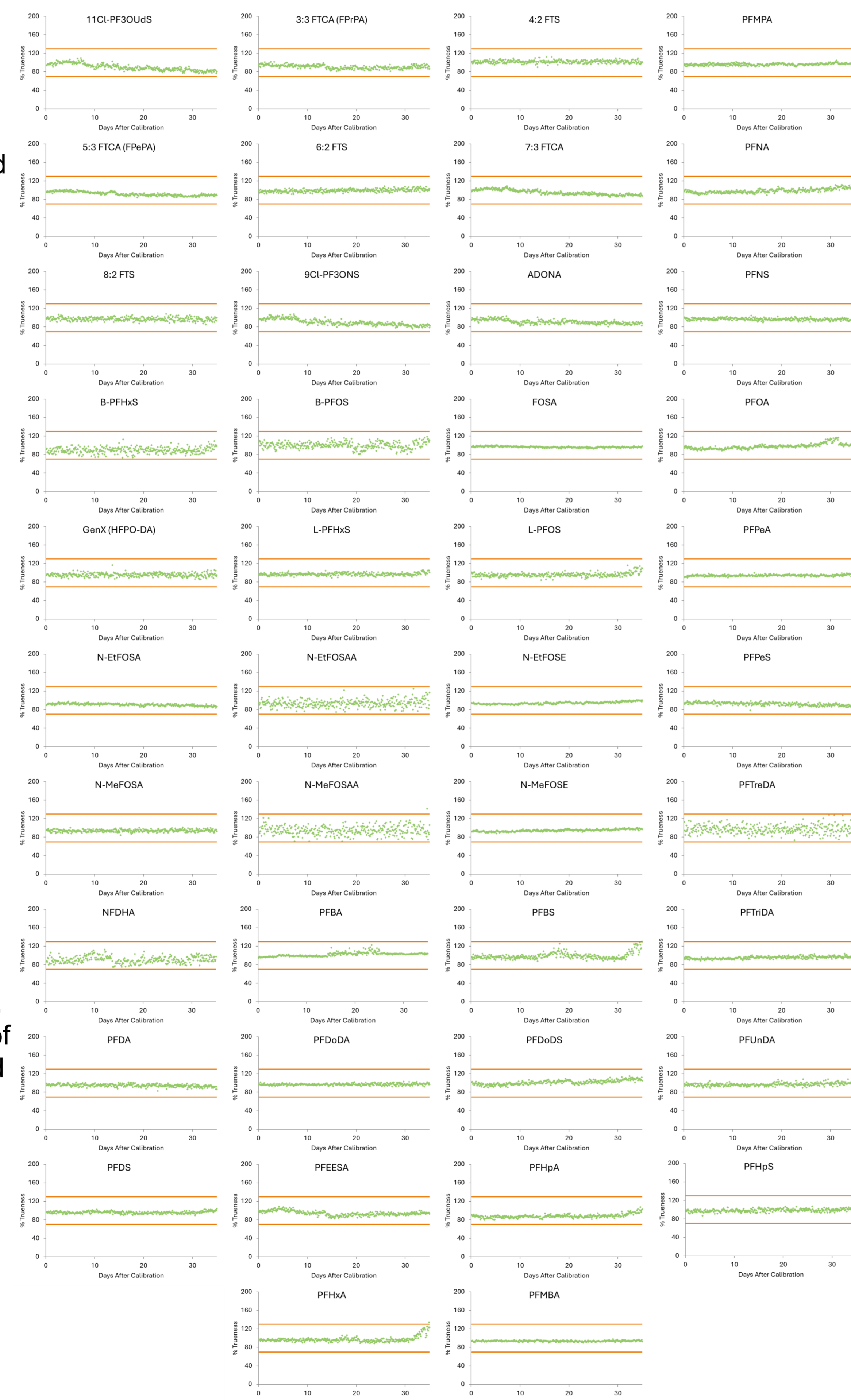


Figure 1. Trueness (%) plots for 42 PFAS with 30% tolerance lines in orange.

Isomer Quantification

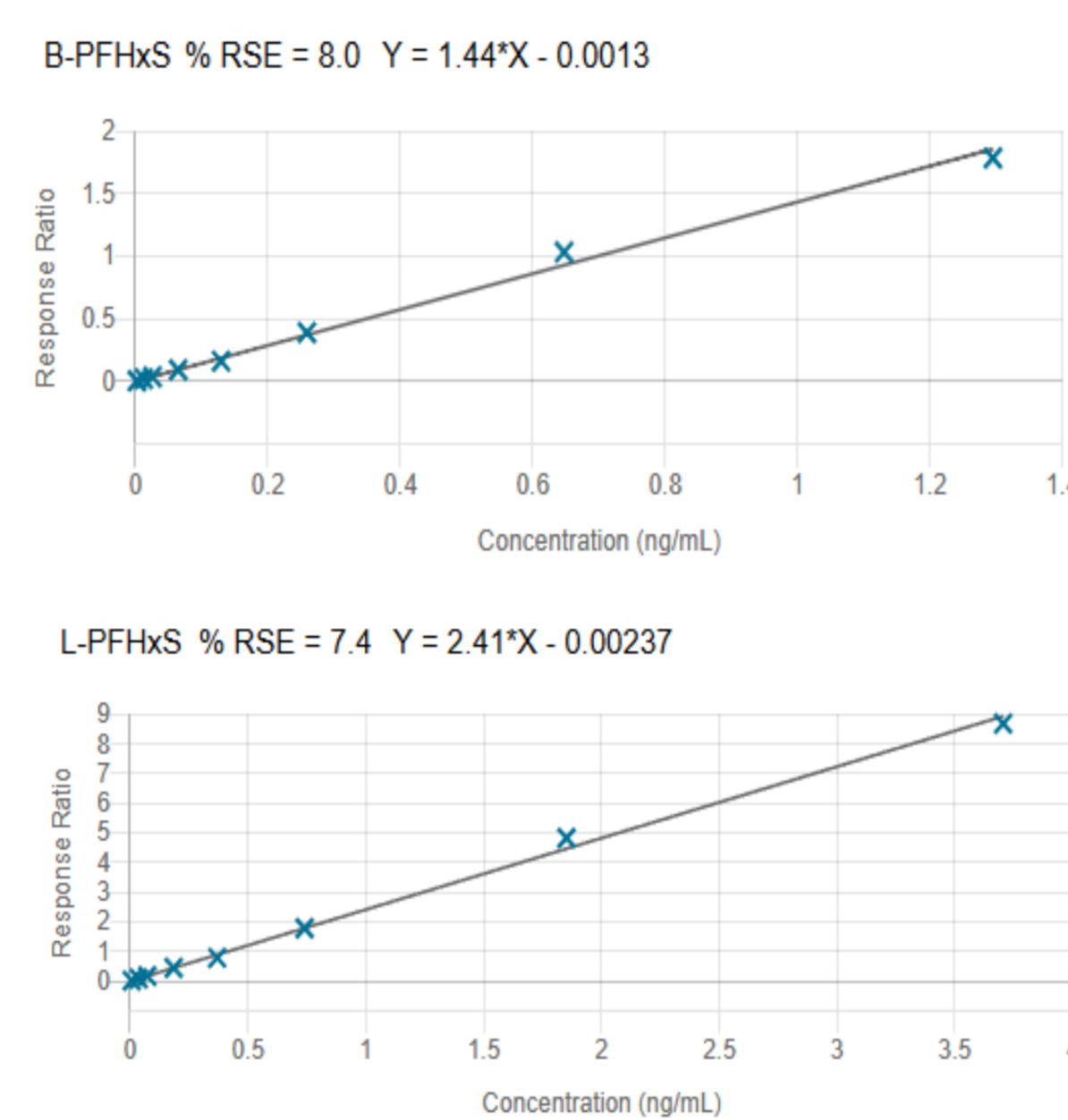


Figure 2. Calibration graphs for branched and linear PFHxS.

PFAS	Mean Conc (ng/mL)	%RSD
L-PFHxS	0.74	1.79%
B-PFHxS	0.34	6.02%
Total PFHxS	1.07	2.31%
L-PFOS	0.29	3.86%
B-PFOS	0.52	5.01%
Total PFOS	0.81	3.75%

Table 1. Data for linear, branched and total PFHxS and PFOS.

For PFOS and PFHxS, separate calibration graphs were successfully applied to branched and linear isomers (Figure 2), with waters_connect for Quantitation Software enabling seamless calculation and reporting of both individual isomer concentrations and total PFAS values. Total concentrations for these analytes remained consistent over the course of the study as shown in Table 1.

Low Mass Confirmation

For some shorter chain PFAS, such as PFBA and PFPeA, it is commonly believed that there is no readily identifiable product ion to use for confirmation. As a result, they typically require the need for a confirmatory run, potentially needing HRMS. However, these compounds do create a m/z 19 product ion from the loss of a fluoride ion that can be detected. The waters_connect for Quantitation Software automatically enhances the transmission of fragments <50 amu to allow sufficient response of this ion over the entire calibration range.

Figure 3 shows the two MRM chromatograms for PFPeA in the landfill leachate extract: one for the quantitation transition (262.90 > 219.00) and one for the confirmation transition (262.90 > 19.00). Both transitions are easy to detect and integrate.

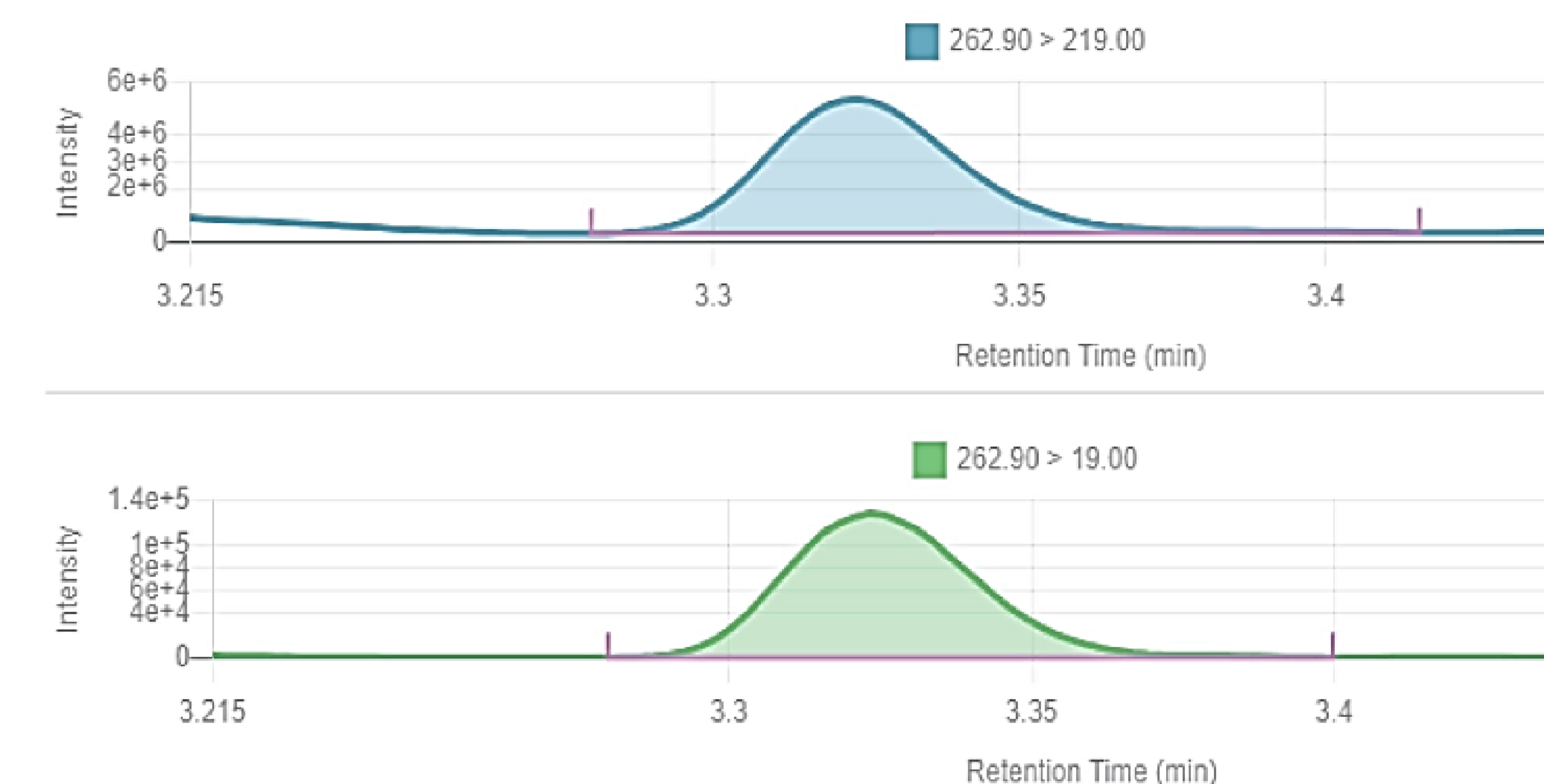


Figure 3. Quantitation (top) and Confirmation (bottom) MRM chromatograms for PFPeA in landfill leachate.

Conclusions

This study demonstrates that the Xevo TQ Absolute XR Mass Spectrometer, operated with waters_connect for Quantitation Software, delivers exceptional robustness, calibration longevity, and analytical confidence for PFAS analysis in complex environmental matrices. Method calibrations remained valid for up to five weeks while meeting trueness and precision criteria, even under demanding, high-throughput conditions involving continuous injections of landfill leachate, biosolids, and surface water extracts. Extended robustness testing confirmed stable quantitation and reporting of branched, linear, and total PFAS isomers, while sensitive detection of low-mass fragment ions enabled reliable confirmation of historically challenging PFAS compounds in a single analytical run. Collectively, these capabilities reduce the need for frequent recalibration, secondary confirmation methods, and unscheduled maintenance, improving laboratory efficiency and reducing consumable costs. By maintaining analytical performance after tens of thousands of injections, the Xevo TQ Absolute XR platform provides testing laboratories with sustained confidence in their PFAS results, supporting regulatory compliance, high sample throughput, and long-term operational reliability.