Application Note

Solving Analytical Challenges in PFAS Testing Using the Xevo TQ Absolute XR Mass Spectrometer with waters_connect for Quantitation

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Published on November 12, 2025

Abstract

Per- and polyfluoroalkyl substances (PFAS) are increasingly monitored due to their persistence and potential environmental impact. Accurate identification, quantification, and confirmation of all components is essential to meet constantly evolving regional reporting requirements. In a robustness study, involving more thanover 17,500 injections on the Xevo™ TQ Absolute XR Mass Spectrometer, landfill leachate samples were analyzed alongside biosolids and river water to assess long-term performance and analytical reliability. Eleven PFAS residues were consistently detected in the leachate extracts, including PFBA and PFPeA—compounds traditionally considered challenging to confirm due to the lack of identifiable product ions for confirmation. However, sensitive detection of the *m/z* 19 product ion enabled reliable confirmation using standard multiple reaction monitoring (MRM) acquisition, facilitated by enhanced low-mass transmission in waters_connect™ for Quantitation Software. Additionally, the Totals feature in waters_connect Software allowed seamless reporting of branched, linear, and total concentrations for PFHxS and PFOS, demonstrating consistent quantitation over 120 days. These findings

highlight the capability of the Xevo TQ Absolute XR Mass Spectrometer and waters_connect for Quantitation Software to deliver robust, high-confidence PFAS analysis without the need for secondary confirmation methods.

Benefits

- Improved instrument uptime when measuring PFAS in a series of challenging matrices so that unscheduled maintenance is minimized
- More control over reporting concentrations of branched and linear PFAS isomers with the Totals feature in waters_connect for Quantitation Software
- Sensitive detection of the *m/z* 19 product ion to provide a confirmation transition for certain analytes that were previously thought to be unconfirmable, allowing quantitation and confirmation in the same injection

Introduction

PFAS testing has become essential in environmental monitoring and in companies relying on accurate results to meet regulatory and quality standards. Accurate identification, quantification, and confirmation using expected retention times, internal standardization, and MRM transition ratios between at least two MRM transitions are prerequisites for successful implementation of official control programs. As part of a robustness study of more than 17,500 injections using the Xevo TQ Absolute XR Mass Spectrometer[1], 30 landfill leachate injections were run every day along with 60 injections from two other challenging matrices (biosolids and river water). Method calibrations were performed using solvent standards. Eleven residues were detected in the leachate extracts, and included 3:3 FTCA, 5:3 FTCA, PFBA, PFBS, PFHpA, PFHxA, PFHxS, PFOA, PFOS, PFPeA, and PFPeS.

Some of the detected analytes, such as PFHxS and PFOS, occur in both branched and linear isomer forms. Since these may degrade differently in the environment, it is important to identify and report them separately and as a total. Regionally, there are differences in reporting requirements for branched and linear PFAS; whether they're reported separately or as a total.

For two of these detected residues, PFBA and PFPeA, it is generally understood that they lack a readily identifiable product ion suitable for confirmation using standard MRM acquisition. As a result, confirmatory analysis may require high-resolution mass spectrometry (HRMS) or alternative approaches, such as a secondary method with a different column.

In this application brief, branched, linear, and total forms of PFHxS and PFOS are successfully identified and reported alongside the successful confirmation of PFPeA in landfill leachate extracts.

Experimental

Landfill leachate (LGC 6177) was purchased as a reference material (without certified PFAS values). Extraction and solid-phase extraction (SPE) clean-up were carried out as outlined in previously published work.[2] In brief, 25 mL landfill leachate was spiked with the extracted internal standard mix. The spiked sample was then loaded onto a conditioned Oasis™ WAX/GCB for PFAS Analysis SPE Cartridge (p/n: 186011110 < https://www.waters.com/nextgen/global/shop/sample-preparation--filtration/186011110-oasis-wax-gcb-for-pfas-analysis-6cc-vac-cartridge-200-mg-wax-50-.html>) at 5 mL/min. The cartridge was washed with 10 mL reagent water followed by 5 mL formic acid/methanol (0.1 M, 1:1 *v/v*) and dried. The extract was eluted with 5 mL ammonium hydroxide in methanol (0.1%, *v/v*). 25 µL acetic acid and the non-extracted internal standard mix was then added to each extract. Five replicates of the landfill leachate samples were extracted and combined prior to analysis. Analysis was carried out on the ACQUITY™ Premier System and Xevo TQ Absolute XR Mass Spectrometer, with both controlled by waters_connect for Quantitation Software as described in previously published work.[1]

Results and Discussion

Branched and Linear Isomers

Separate calibration graphs were plotted for branched and linear PFHxS and PFOS, with waters_connect Software offering the option to report these isomers as a total (Figure 1).

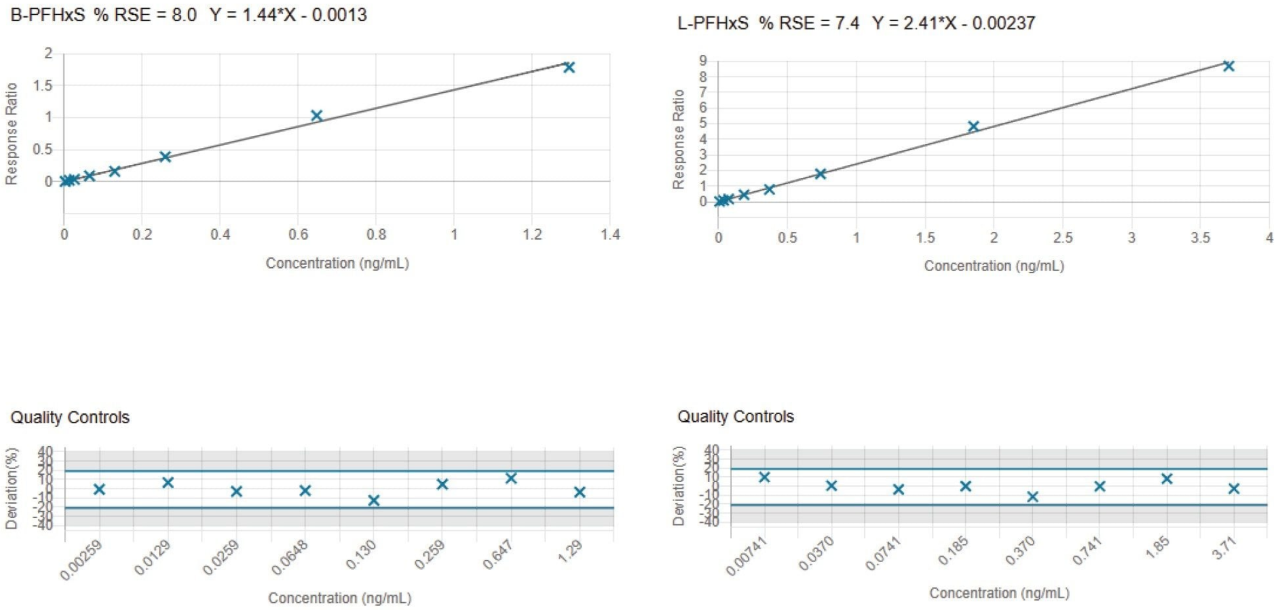
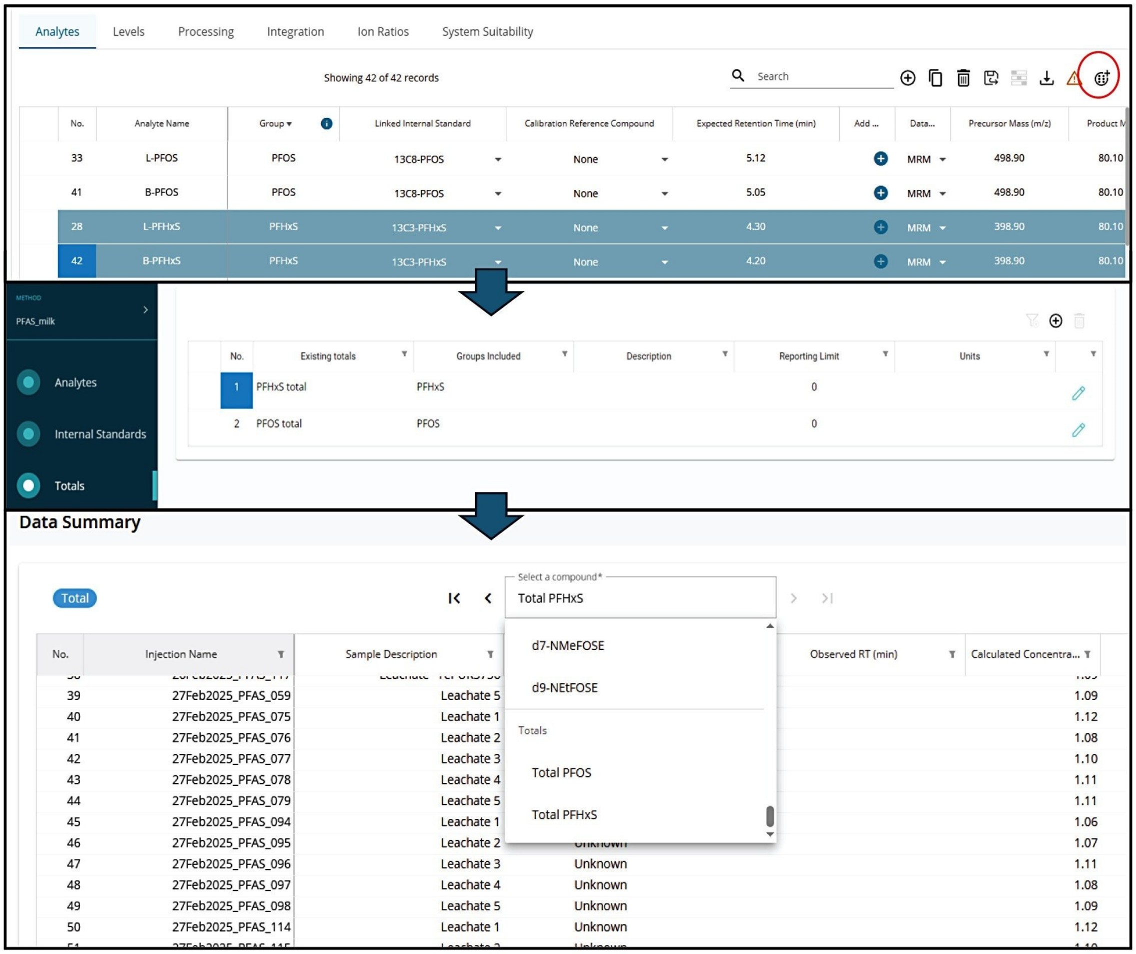


Figure 1. Calibration graphs for branched and linear PFHxS.

Figure 2 shows the workflow for obtaining total concentrations for separate isomers. Transitions of isomers are labelled as a group, then the Totals tab pulls the data from the desired group and sets parameters like units and reporting limit.



No.	Analyte Name	Group	Linked Internal Standard	Calibration Reference Compound	Expected Retention Time (min)	Add ...	Data...	Precursor Mass (m/z)	Product M
33	L-PFOS	PFOS	13C8-PFOS	None	5.12	⊕	MRM	498.90	80.10
41	B-PFOS	PFOS	13C8-PFOS	None	5.05	⊕	MRM	498.90	80.10
28	L-PFHxS	PFHxS	13C3-PFHxS	None	4.30	⊕	MRM	398.90	80.10
42	B-PFHxS	PFHxS	13C3-PFHxS	None	4.20	⊕	MRM	398.90	80.10

No.	Existing totals	Groups Included	Description	Reporting Limit	Units	
1	PFHxS total	PFHxS		0		
2	PFOS total	PFOS		0		

No.	Injection Name	Sample Description		Observed RT (min)	Calculated Concentra...
39	27Feb2025_PFAS_059	Leachate 5			1.09
40	27Feb2025_PFAS_075	Leachate 1			1.12
41	27Feb2025_PFAS_076	Leachate 2			1.08
42	27Feb2025_PFAS_077	Leachate 3			1.10
43	27Feb2025_PFAS_078	Leachate 4			1.11
44	27Feb2025_PFAS_079	Leachate 5			1.11
45	27Feb2025_PFAS_094	Leachate 1			1.06
46	27Feb2025_PFAS_095	Leachate 2			1.07
47	27Feb2025_PFAS_096	Leachate 3	Unknown		1.11
48	27Feb2025_PFAS_097	Leachate 4	Unknown		1.08
49	27Feb2025_PFAS_098	Leachate 5	Unknown		1.09
50	27Feb2025_PFAS_114	Leachate 1	Unknown		1.12

Figure 2. The 'Totals' workflow within MS Quan in waters_connect for Quantitation.

The results for each isomer and the total can be found in the data summary page. Branched, linear, and total concentrations were calculated for PFOS and PFHxS for more than 4000 leachate extract injections and exhibited consistent data as shown in Table 1.

PFAS	Mean Concentration (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.

Using m/z 19 as a Product Ion for Confirmation

For smaller 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. For official control, this removes the requirement for HRMS or a second confirmatory run using a different column, allowing quantitation and confirmation in a single injection. Figure 3 shows the two MRM chromatograms for PFPeA in the leachate extract: one for the quantitation transition (262.90 > 219.00) and one for the confirmation transition (262.90 > 19.00). Both transitions are being easy to detect and integrate.

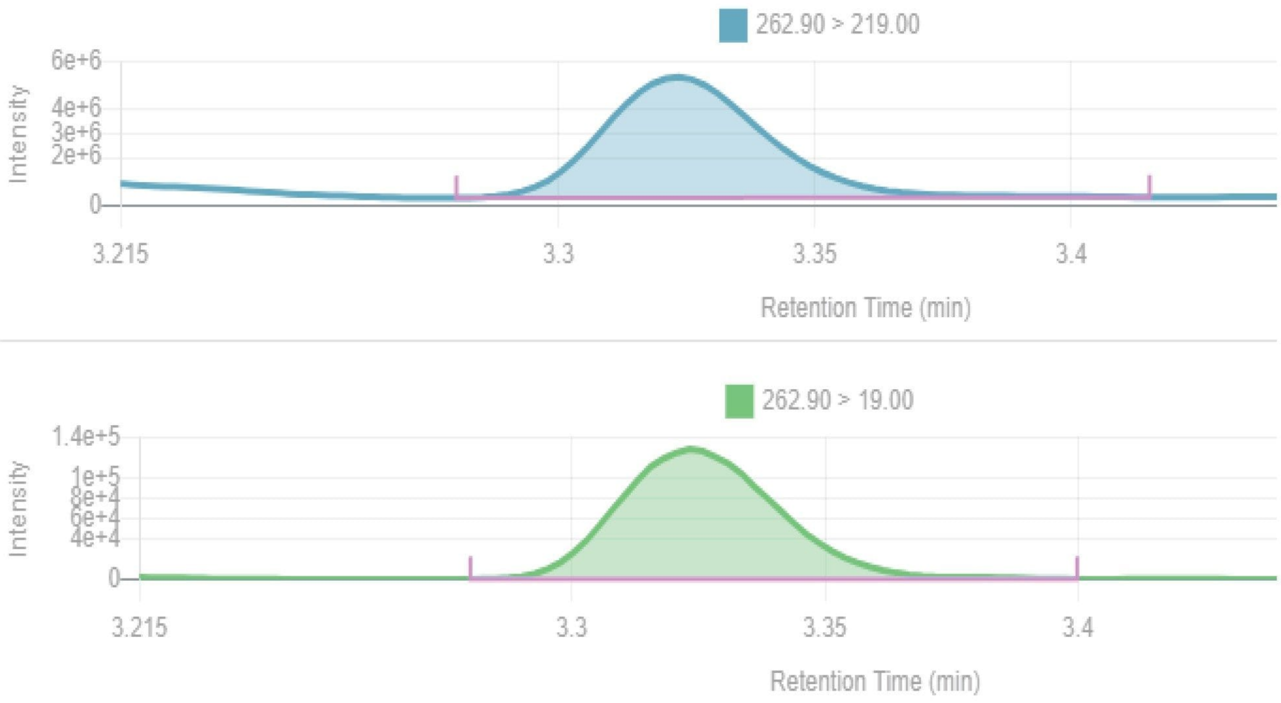


Figure 3. Quantitation (top) and Confirmation (bottom) MRM chromatograms for PFPeA in leachate.

Figure 4 shows a plot of the confirmation/quantitation ion ratio from the same injection on each day of the study, with the expected ion ratio being consistently maintained over a 120-day period, with a ±30% tolerance based on the average of the first 50 results.

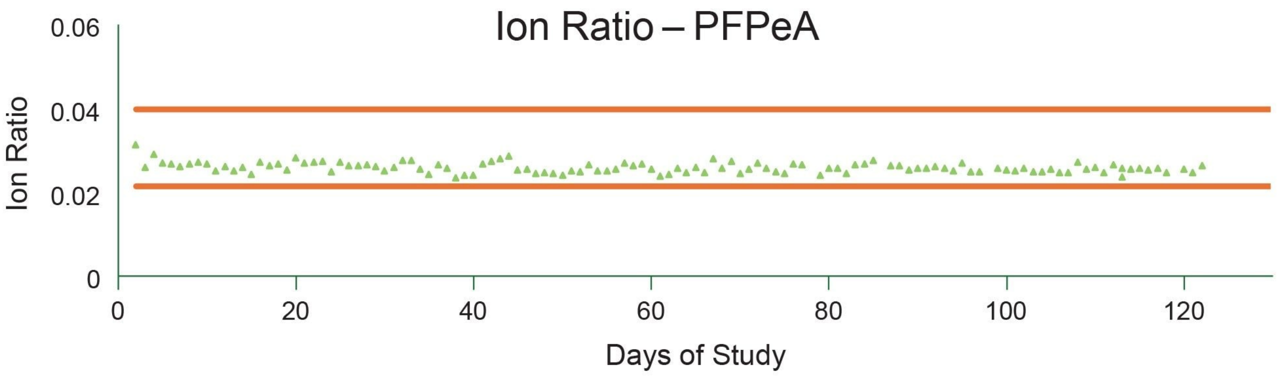


Figure 4. Ion ratio of PFPeA using the m/z 19 product ion over 120 days of the study.

Conclusion

Accurate identification, quantification, and confirmation of PFAS are prerequisites for successful implementation of official control programs.

As part of a PFAS robustness study using several challenging matrices, the ACQUITY Premier System and Xevo TQ Absolute XR Mass Spectrometer, with both controlled by waters_connect for Quantitation Software, were able to provide consistently accurate data on landfill leachate extracts over the course of 120 days.

The Totals feature within MS Quan in waters_connect for Quantitation Software allows lab users to report analytes with branched and linear isomer forms as separate and total concentrations.

The ability of the waters_connect for Quantitation Software to enable sensitive and accurate detection of the *m/z* 19 product ion gives confidence in measurements of difficult analytes like PFPeA and PFBA, and removes the need for confirmatory runs on HRMS or a second confirmatory run using a different column.

References

1. Hancock P, Adams S, Gould D. Enhanced Reliability for Long-Term PFAS Analysis with the Xevo TQ Absolute XR Mass Spectrometer, Waters Application Note. 720008824.
2. Organtini KL, Rosnack KJ, Plummer C, Hancock PM, Burt O. Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Accordance with EPA 1633 Part 2: Analysis of Aqueous Matrices. Waters Application Note. 720008143.

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720009126, November 2025