アプリケーションノート

Ensuring Safe and Affordable Drinking Water in the United Arab Emirates (UAE) Market Through Per- and Polyfluoroalkyl Substances (PFAS) Testing using the ACQUITY™ UPLC™ I-Class and Xevo™ TQ Absolute System

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Application Brief

This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief highlights an advanced analysis of per- and polyfluoroalkyl substances (PFAS) in bottled drinking water, helping ensure safe and affordable water for communities across the UAE. The method is aligned with the PFAS sum parameter listed in the EU Drinking Water Directive (EU DWD) 2020/2184.[1] To allow high-throughput, a previously published PFAS method[2] was reduced from 22 minutes run time to 15 minutes. Leveraging a streamlined dilute-and-shoot workflow, the ACQUITY UPLC I-Class Plus System combined with the

Xevo TQ Absolute Mass Spectrometer delivers unmatched sensitivity. Together, they enable ultra-trace quantitation at parts-per-trillion (ppt; ng/L) levels, providing the precision and reliability needed to meet stringent regulatory standards and safeguard public health.[3]

Benefits

- Dilute-and-shoot sample preparation offers a fast, cost-effective, and reproducible workflow by minimizing handling steps, reducing contamination risk, and enabling high-throughput analysis with reliable accuracy.
- Comprehensive screening and quantification of the 27 most prevalent PFAS analytes achievable in a single injection is in alignment with the EU (EU DWD).
- A previously published method providing the highest sensitivity was optimized towards UAE requirements in terms of relevant PFAS compounds and throughput.

Introduction

PFAS employed in applications ranging from non-stick coatings and surfactants to food packaging, fire-fighting foams, and as polymerization aids for polytetrafluoroethylene (PTFE) and other fluoropolymers, exhibit remarkable chemical stability and environmental persistence. Most of these compounds are bioaccumulative and have been detected in human blood, underscoring their pervasive impact on both ecosystems and public health.[4]

Monitoring PFAS in drinking water is critical because they are widespread, resistant to natural breakdown, and linked to serious health risks, including cancer, immune dysfunction, and developmental issues. With thousands of distinct compounds, PFAS are widely used across consumer, commercial, and industrial applications. Their sheer diversity and widespread use complicate efforts to investigate and evaluate the potential risks they pose to human health and the environment.

This application brief outlines an adapted analytical methodology from the previously published application note by Waters[2] for the determination of 27 PFAS compounds in alignment with the EU DWD to monitor bottled drinking water in the UAE. The approach employs a streamlined dilute-and-shoot technique, leveraging the exceptional sensitivity and performance of the ACQUITY UPLC I-Class System in combination with the Xevo TQ Absolute Mass Spectrometer. By eliminating labor-intensive preconcentration procedures, the likelihood of analyte loss or sample contamination is substantially reduced, while simultaneously enhancing sample throughput and analytical efficiency, thereby reducing overall costs.

With the number of analytes reduced to 27 PFAS compounds, the method could be further optimized, allowing the overall analysis time to be shortened from 22 minutes to 15 minutes. This reduction not only enhances high-throughput capacity but also facilitates more rapid and reliable monitoring of PFAS in drinking water.

Results and Discussion

To minimize sample preparation, conserve time, and mitigate the risk of contamination, a straightforward dilute-and-shoot strategy was employed. Bottled drinking water was diluted 1:1 with acidified methanol, vortex mixed, and subsequently transferred into polypropylene vials for direct injection of 50 µL of sample. Based on the previously published application note[2] (p/n: 720008137 < https://www.waters.com/nextgen/global/library/application-notes/2023/extending-pfas-coverage-and-sensitivity-in-a-direct-injection-uplc-msms-method-for-water-matrices-based-on-eu-and-uk-drinking-water-regulations.html>), the overall run time of the LC method was reduced to 15 minutes, maintaining a good separation of all PFAS compounds (Figure 1).

The mass spectrometer parameters described in the application note were further optimized for this study. Under negative electrospray ionization mode, the capillary voltage was set to 0.5 kV. As no thermolabile PFAS compounds were included in the analytical panel, the source temperature was elevated from 110 °C to 130 °C, while the desolvation temperature was increased from 400 °C to 500 °C.

The acquisition was performed using MassLynx™ 4.2 Software, while data processing of 27 PFAS compounds was carried out in waters_connect™ for Quantitation Software. The exception focused review functionality facilitates a faster and more efficient evaluation of large datasets, streamlining the overall analytical workflow.

With the exceptional sensitivity of the Xevo TQ Absolute and the optimized mass spectrometer parameters, a limit of quantitation (LOQ) of 1 ng/L and calibration curves ranging from 1 to 250 ng/L were achieved for all 27 PFAS. All MRM conditions with cone and collision energies are listed in Table 1.

Analyte	ESI mode	Precursor Ion (*m/z*)	Quantifier Ion/ Qualifier ion (*m/z*)	Cone voltage (V)	Collision energy (CV)
PFBA	neg	212.90	169.00	10	10
			–		–
PFPeA	neg	262.90	219.00	10	5
			–		–
PFHxA	neg	312.90	269.00	5	10
			119.00		20
PFHpA	neg	362.90	319.00	15	10
			169.00		15
PFOA	neg	412.90	369.00	10	10
			169.00		15
PFNA	neg	462.90	418.90	10	10
			219.00		15
PFDA	neg	512.90	468.90	15	15
			219.00		15
PFUnDA	neg	562.90	518.90	25	10
			269.00		20
PFDoDA	neg	612.90	568.90	30	25
			169.00		10
PFTriDA	neg	662.90	618.90	5	10
			169.00		30
PFTreDA	neg	712.90	668.90	10	15
			169.00		25
PFBS	neg	298.90	80.10	15	30
			99.10		30
PFPeS	neg	348.90	80.10	10	30
			99.10		30
PFHxS	neg	398.90	80.10	10	35
			99.10		35
PFHpS	neg	448.90	80.20	15	35
			99.10		35
PFOS	neg	498.90	80.20	15	40
			99.10		40
PFNS	neg	548.90	80.20	20	40
			99.20		40
PFDS	neg	598.90	80.20	25	40
			99.10		40
11Cl-PF3OUdS	neg	630.90	450.80	30	30
			83.00		30
9Cl-PF3ONS	neg	530.90	350.90	15	25
			83.00		25
4:2 FTS	neg	326.90	81.10	15	35
			307.00		15
6:2 FTS	neg	426.90	81.00	15	35
			407.00		10
8:2 FTS	neg	526.90	81.20	15	40
			506.80		10
ADONA	neg	376.90	251.00	10	10
			85.00		25
FOSA	neg	497.90	78.20	40	30
			169.20		30
N-EtFOSAA	neg	584.00	418.80	15	20
			525.90		20
N-MeFOSAA	neg	569.90	418.90	35	20
			219.10		25

Table 1. MRM transitions, collision energies, and cone voltages for 27 PFAS compounds.

The optimized method demonstrated outstanding linearity and high reproducibility across the 27 selected PFAS compounds. As illustrated in Figure 1, chromatographic separation was achieved for all analytes, with elution times under 10 minutes.

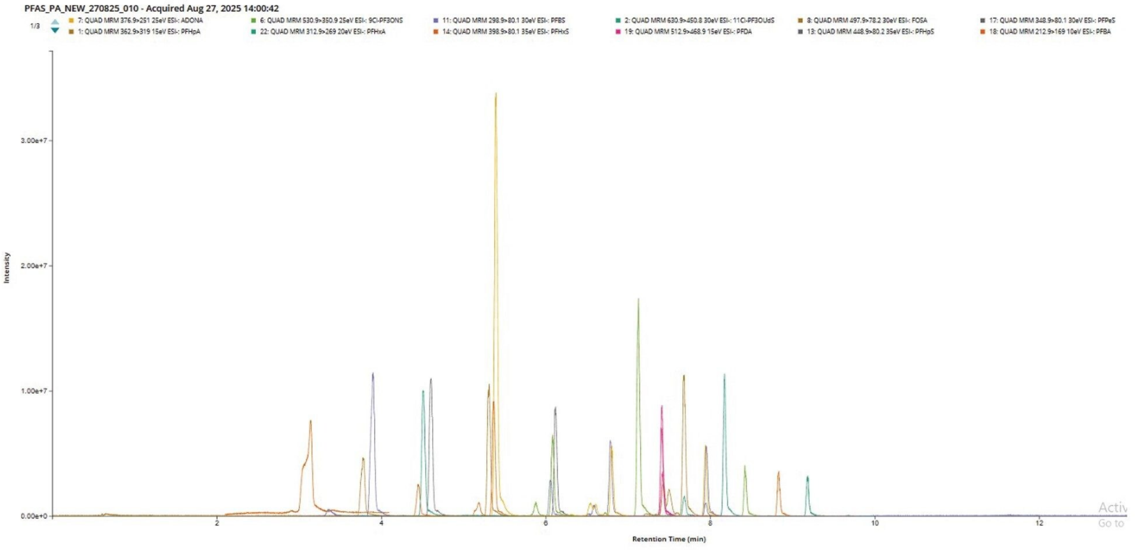


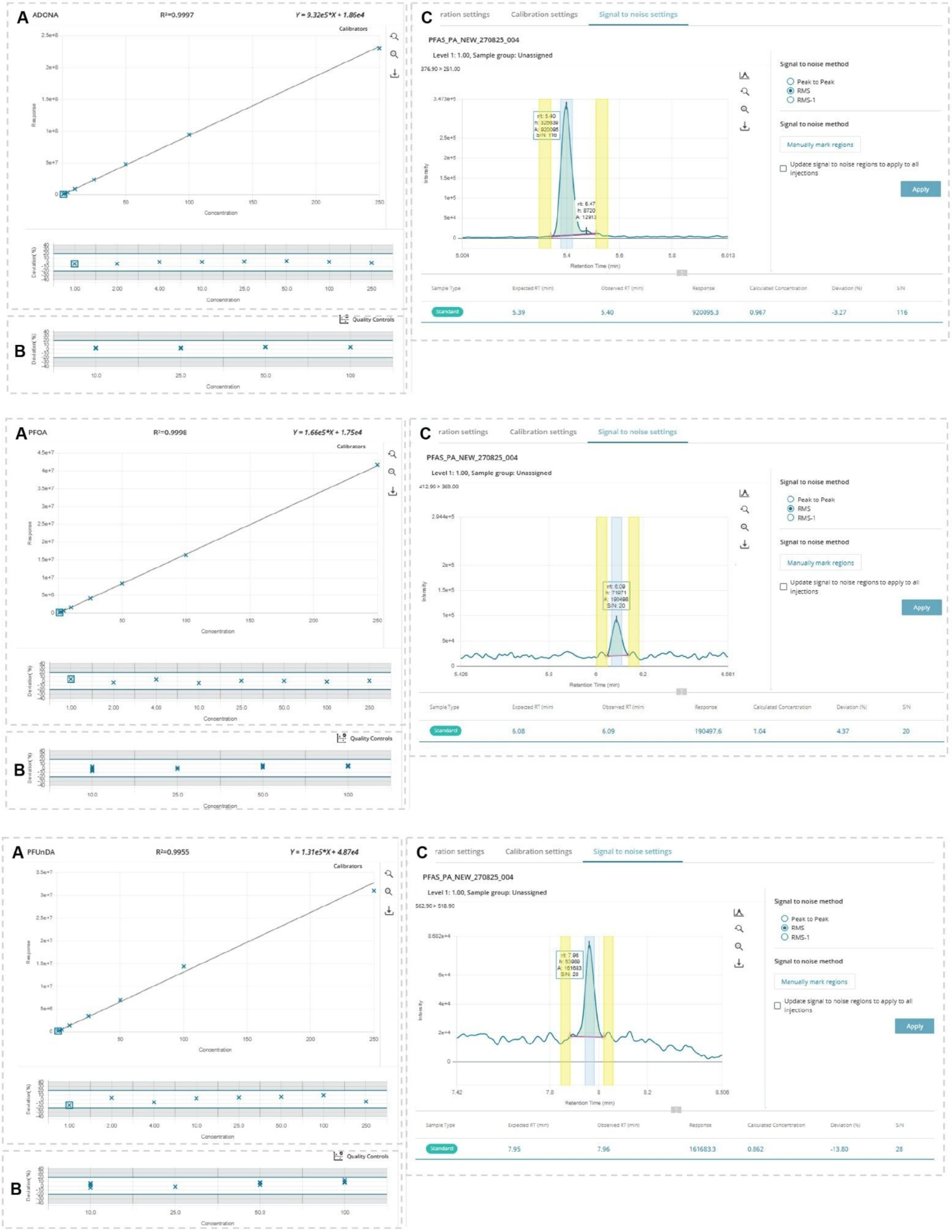
Figure 1. Chromatographic elution pattern for 27 PFAS compounds within 10 minutes.

Figure 2 shows linear calibration curves for selected PFAS compounds, ranging from 1 to 250 ng/L, demonstrating both the sensitivity and dynamic range of the system. For each compound, the percentage deviation of each individual calibration standard is well within a 20% deviation range (Figure 2, A). All 11 drinking water samples tested with this approach showed no detectable PFAS contamination.

To assess reproducibility, three of these water samples were pooled and spiked at four different concentration levels (10, 20, 50, and 100 ng/L). Repeated injections demonstrated strong system reproducibility, with QC deviations remaining well within the 20% tolerance (Figure 2, B).

In addition, Figure 2 shows the calculated signal-to-noise ratios for the PFAS compounds at 1 ng/L (Figure 2, C), highlighting the method's capability for ultra-trace quantitation.

The PFAS compounds displayed in Figure 2 were chosen to represent a range of classes, spanning well-known perfluorooctanoic acid (PFOA) to long-chain perfluoroundecanoic acid (PFUnDA) species, as well as emerging PFAS 4,8-dioxa-3H-perfluorononanoic acid (ADONA).



PFAS_PA_NEW_270825_004

Level 1: 1.00, Sample group: Unassigned

376.90 > 251.00

Signal to noise method

○ Peak to Peak
● RMS
○ RMS-1

Signal to noise method

Manually mark regions

☐ Update signal to noise regions to apply to all injections

Sample Type	Expected RT (min)	Observed RT (min)	Response	Calculated Concentration	Deviation (%)	S/N
Standard	5.39	5.40	920095.3	0.967	-3.27	116

PFAS_PA_NEW_270825_004

Level 1: 1.00, Sample group: Unassigned

412.90 > 369.00

Signal to noise method

○ Peak to Peak
● RMS
○ RMS-1

Signal to noise method

Manually mark regions

☐ Update signal to noise regions to apply to all injections

Sample Type	Expected RT (min)	Observed RT (min)	Response	Calculated Concentration	Deviation (%)	S/N
Standard	6.08	6.09	190497.6	1.04	4.37	20

PFAS_PA_NEW_270825_004

Level 1: 1.00, Sample group: Unassigned

562.90 > 518.90

Signal to noise method

○ Peak to Peak
● RMS
○ RMS-1

Signal to noise method

Manually mark regions

☐ Update signal to noise regions to apply to all injections

Sample Type	Expected RT (min)	Observed RT (min)	Response	Calculated Concentration	Deviation (%)	S/N
Standard	7.95	7.96	161683.3	0.862	-13.80	28

Figure 2. A: Calibration information (1 to 250 ng/L), B: QC deviations of 4 QC levels (10, 20, 50, and 100 ng/L), and C:

Calculated signal-to-noise values at 1 ng/L for three exemplarily selected PFAS: PFOA, PFUnDA, and ADONA.

Recoveries of PFAS compounds in an exemplary matrix derived from 3 pooled drinking water samples were consistently within the tolerable range of 120 to 70%, ranging from 84% to 105% at the lowest quality control (QC) level of 10 ng/L. These results demonstrate the robustness and accuracy of the method even at trace concentrations, ensuring reliable quantification of PFAS in compliance with stringent analytical performance criteria.

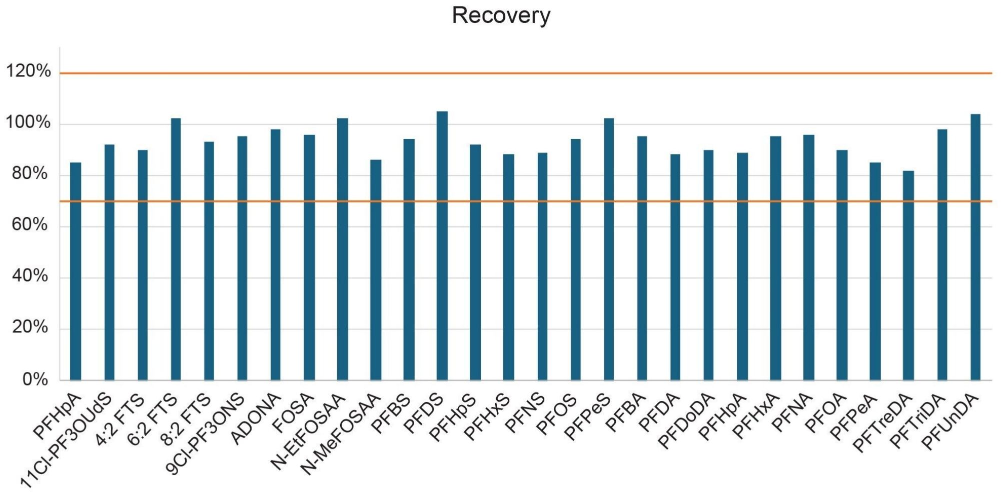


Figure 3. Recovery of PFAS compounds from pooled drinking water samples ranged from 84% to 105% at the lowest QC level (10 ng/L). Orange bars indicate the upper and lower tolerance for recoveries.

Conclusion

This application brief presents an optimized LC-MS/MS method for the analysis of 27 PFAS compounds aligned with EU DWD regulations. The use of a straightforward dilute-and-shoot approach combined with a reduced LC runtime of 15 minutes enables rapid and convenient monitoring of PFAS at trace-level concentrations in drinking water in the UAE. The method delivers exceptional sensitivity with an LOQ of 1 ng/L and a broad dynamic range, demonstrating linearity from 1 to 250 ng/L for all 27 PFAS.

Quality control samples from pooled drinking water confirmed excellent reproducibility and recovery. All 11 bottled water samples analyzed with this method showed no PFAS contamination above the quantification limit which is set at regulatory requirements. Enhanced negative ion sensitivity of the Xevo TQ Absolute, together with optimized mobile phase composition and source parameters, ensure consistent performance at sub-ng/L detection limits throughout the study. These capabilities support high-throughput drinking water analysis, enabling timely and reliable monitoring to safeguard public health.

References

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