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Note d'application

Expanding the Range of PFAS in a Single Injection to Include Ultra Short Chains Using the Atlantis™ BEH™ C_{18} AX Mixed Mode Column

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Abstract

As the legacy long chain PFAS were voluntarily phased out of production, they were replaced by short and ultra-short chain PFAS of similar chemistries. Chromatography methods using common reverse phase columns do not retain the ultra-short PFAS, so these are not usually included in quantitative methods. The mixed mode chemistry of PFAS molecules, both hydrophobic and ionic, should be retained on mixed mode reverse phase and anion exchange column chemistries such as the Atlantis Premier BEH C_{18} AX Column. TFA, PFPrA, and PFPrS were sufficiently retained using the Atlantis Premier BEH C_{18} AX Column and can be analyzed and quantified in the same method as the legacy long chain PFAS compounds. A wide variety of water samples were evaluated on the mixed mode column with TFA, PFPrA, and PFPrS detected in significant quantities in a landfill leachate sample. Use of the Atlantis Premier BEH C_{18} AX Column now broadens the scope of PFAS that can be routinely detected and quantified in a single injection to include the ultra-short chain PFAS down to C2 carbon chain length.

Benefits

- A single method that broadens the scope of PFAS compounds to now include analysis of C2 through C14 chain length PFAS by utilizing the mixed mode (hydrophobic and ionic) nature of the compounds
- Improvements in chromatographic retention and peak shape of ultra-short and short chain PFAS on the Atlantis Premier BEH C_{18} AX Column allows for fewer manual peak integrations
- Accurate quantitative results for 46 PFAS in authentic matrix samples, verified by an ERA wastewater matrix certified reference material in order to assess reporting reliability

Introduction

When the environmental impact and health hazards of the legacy long-chain (≥C8) PFAS were realized, a shift in manufacturing was made to substitute their use with short chain (C4–C7) and ultra-short chain (≤C3) PFAS.[1] Initially it was believed that these substituted short and ultra-short chain PFAS would have less environmental and health impacts, but it has been shown that they are highly mobile in the environment, degrade to very persistent end products, and still pose significant health concerns.[2] In order to get a broader, more accurate representation of PFAS contamination, one may expect expanded coverage in regulatory methods, requiring methods that can easily and accurately quantify the ultra-short chain compounds. However, many of the current PFAS regulations and standard methods don't include PFAS in the ultra-short chain category. A summary of the common global methods and regulations currently in place for PFAS are listed in Table 1 with the short and ultra-short chain PFAS that are included in each method. This summary demonstrates that it is uncommon for methods to include PFAS in chain length less than C4, other than the ASTM 8421 that includes perfluoropropionic acid (PFPrA). Even though the ultra-short chain PFAS are often not included in routine PFAS methods, it does not mean they are not found in common samples. For instance, a 2019 study by Bjornsdotter et al. identified ultra-short chain PFAS such as trifluroracetic acid (TFA) and perfluoropropanesulfonic acid (PFPrS) in Swedish water samples at 14,000 and 15,000 ng/L, respectively.[3] Additionally, it has been shown that the ultra-short chain PFAS can account for a portion of the unknown total fluorine content of samples as concluded by a 2021 study by Aro et al. In this study a total of 10% of fluorine content in wastewater samples could be identified, amongst which 4% was identified as ultra-short chain PFAS.[4] Excluding ultra-short chain PFAS from routine quantitative methods can lead to a significant underrepresentation of PFAS present in samples.

Method/ regulation	TFA (C2)	PFPrA (C3)	PFBA (C4)	PFPeA (C5)	PFHxA (C6)	PFHpA (C7)	PFPrS (C3)	PFBS (C4)	PFPeS (C5)	PFHxS (C6)	PFHpS (C7)
EPA 537.1					x	x		x		x	
EPA 533			x	x	x	x		x	x	x	x
EPA 1633			x	x	x	x		x	x	x	x
EU 2020/2184			x	x	x	x		x	x	x	x
EU 2022/2388										x	
ISO 21675			x	x	x	x		x		x	x
ASTM 8421		x	x	x	x	x		x	x	x	x

Table 1. Overview of ultra-short and short chain PFAS that are included in current methods and regulations.

As PFAS use and manufacturing has evolved, one possible reason that the ultra-short chain PFAS may not be included in routine PFAS methods is because of the difficulties with chromatographing these small compounds. PFAS analysis is most commonly performed using a reverse phase column, most typically a C_{18} chemistry. The hydrophobic C-F chain on PFAS molecules allows for the retention and separation mechanism to work under these conditions. However, as the C-F chain length decreases, the ability for hydrophobic retention on the C_{18} chemistry decreases. Typical C_{18} based methods have PFBA eluting fairly close to the void volume of the column, indicating that it is just barely retained. Besides the hydrophobic chemistry of the C-F chain, most PFAS also have a negatively charged ionic head group, which provides a secondary retention mechanism that could be used. The Atlantis Premier BEH C_{18} AX Column combines both the reverse phase C_{18} and anion exchange (AX) retention chemistries into one column. In this case, a mixed mode column can take advantage of both portions of the PFAS compounds. Reverse phase and anion exchange combined together is already commonly used for PFAS sample preparation when utilizing solid phase extraction (SPE) in the format of weak anion exchange (WAX) based cartridges. In this application of mixed mode chemistries, the anion exchange portion is important for retaining the short chain PFAS as they have a weaker reverse phase mechanism than the long chain PFAS.

In this work, the mixed mode chemistry column, Atlantis Premier BEH C_{18} AX Column, was evaluated to determine how short and ultra-short chain PFAS could be retained on this column and if it could be used for routine PFAS analysis of ultra-short through long chain PFAS.

Experimental

Sample Preparation

Water samples analyzed were provided by US EPA Region 5. Water samples were collected in the following locations: landfill leachate, a metal finisher, wastewater effluent, wastewater influent, hospital discharge, a bus washing station, a powerplant, pulp and paper factory, ground water, and surface water. A wastewater certified reference material from ERA (item number 404 <https://www.eraqc.com/pfas-in-wastewater-wp-era001663?returnurl=%2fsearch%3fq%3d404>) was also analyzed alongside the collected water samples to evaluate the method performance using a certified material.

Water samples were prepared in accordance with the ASTM 8421 method.[5] The entirety of each 5 mL water sample was used to avoid any compound loss from subsampling. Each sample was spiked with 160 ng/L of isotopically labeled surrogates. 5 mL methanol was then added to each water sample and vortexed. The entire 10 mL sample was syringe filtered using a 25 mm, 0.2 µm polypropylene syringe filter. Following filtration, 10 µL acetic acid was added to each sample. Additional acetic acid was added to samples that had a pH > 4, as needed. An aliquot of each sample was transferred to a polypropylene autosampler vial for analysis on the Xevo™ TQ Absolute MS coupled to an ACQUITY™ I Class FTN BSM System modified with a PFAS Kit.

Data Review

The data generated using the Atlantis Premier BEH C_{18} AX Column was evaluated against the data quality guidelines outlined in ASTM 8421, which included the following:

1. A minimum 5-point linear calibration curve must be utilized.

2. Deviation (% error) of calibration standards and QC injections must be 30% of the expected concentration.

3. Blank response must be <50% of response of the LLOQ injection.

4. Internal standard response must be within 30% of the median response of the batch.

5. Internal standard and native retention time must be within 5% (+/- 3 sec) of the expected retention time.

6. Ion ratios must be within 30% of the mean reference peaks.

LC Conditions

LC system:	ACQUITY I Class BSM with FTN

Vials:	700 µL Polypropylene Screw Cap Vials (p/n: 186005219)
Analytical column:	Atlantis Premier BEH C_{18} AX 2.1 x 100 mm, 1.7 µm (p/n: 186009368)
Isolator column:	Atlantis Premier BEH C_{18} AX 2.1 x 50 mm, 2.5 µm (p/n: 186009390)
Column temperature:	35 °C
Sample temperature:	10 °C
Injection volume:	30 µL
Flow rate:	0.3 mL/min
Mobile phase A:	2 mM ammonium acetate in water
Mobile phase B:	0.1% (v/v) ammonium hydroxide in methanol

Gradient Table

Time (min)	%A	%B	Curve
0	99	1	initial
2	99	1	6
3	75	25	6
8	50	50	6
15	15	85	6
16	0	100	6
20	0	100	6
20.1	100	0	6
23.5	100	0	6
24	99	1	6

MS Conditions

MS system:	Xevo TQ Absolute
Ionization mode:	ESI-
Capillary voltage:	0.5 kV
Source temperature:	100 °C
Desolvation temperature:	350 °C
Desolvation flow:	900 L/hr
Cone flow:	150 L/hr

MRM method:	See Appendix for Full MRM Method details

Data Management

Software:	waters_connect™ for Quantitation

Results and Discussion

Prior to availability of a mixed mode chromatography column, the reverse phase mechanism (C_{18}) has been primarily used to perform PFAS analysis.[6] PFAS from the carboxylic acid family with chain lengths below C4 are not sufficiently retained on standard reverse phase columns, as shown in the top chromatogram of Figure 1. In this example, TFA (C2) and PFPrA (C3) elute within the void region (T_0) of the column. This distorts peak shape, as seen with PFPrA, but also significantly increases the chance of matrix interference from the unretained matrix compounds that also elute in this region. With the mixed mode Atlantis Premier BEH C_{18} AX Column having both reverse phase and anion exchange mechanisms, the hydrophobicity of the C-F chain isn't the only mode of retention for PFAS. The functional group, such as $-CO_2$ or $-SO_4$, also plays a role in retention, allowing for increased retention of the ultra-short chain PFAS like TFA and PFPrA where the C-F chain is not as hydrophobic as the longer chain PFAS. The bottom chromatogram in Figure 1 demonstrates the increased retention of the ultra-short chain PFAS on the Atlantis Premier BEH C_{18} AX Column utilizing the gradient described in this work. Although TFA was retained on the mixed mode column, there was still a large TFA contamination present within samples prepared in the laboratory, which is a shared use laboratory where other applications are using TFA as a mobile phase modifier. This makes TFA contamination in samples and standards difficult to control. Therefore, chromatograms shown in this application note use the isotope labelled TFA analog as the representative peak for TFA.

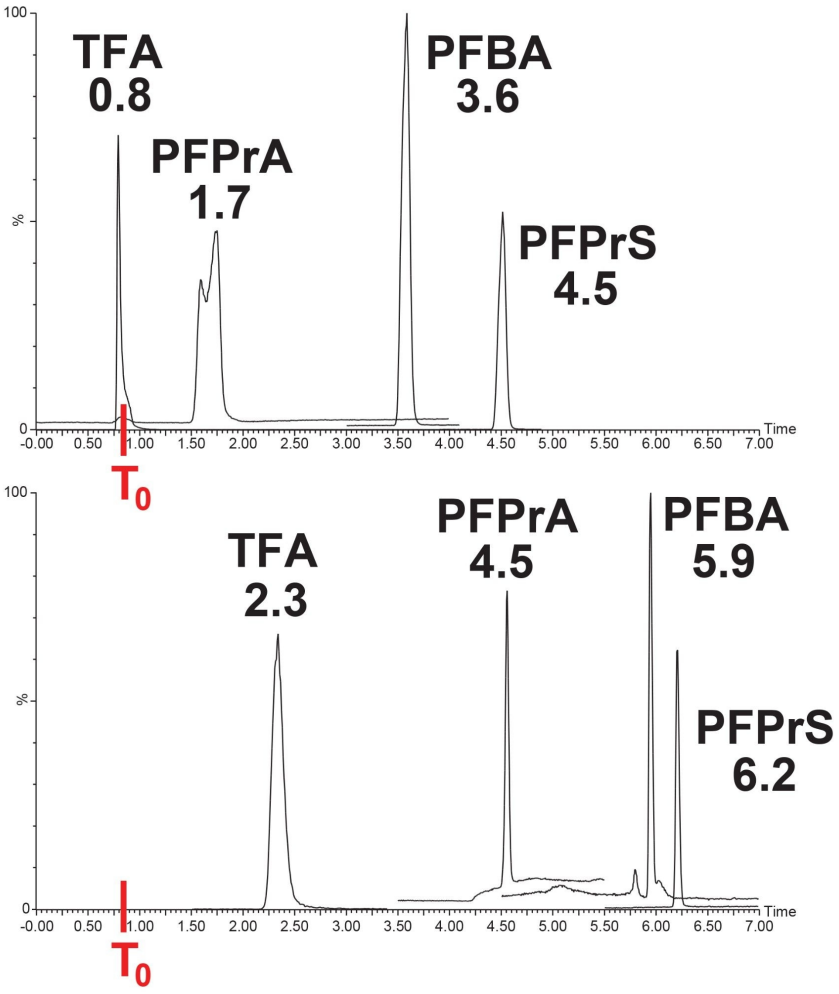

Figure 1. Retention comparison of TFA, PFPrA, PFBA, and PFPrS, labelled with retention times, on a reverse phase only column (top) and the mixed mode Atlantis Premier BEH C_{18} AX Column (bottom). TFA is represented using an isotope labelled analog of TFA due to contamination issues with the native TFA analog.

Standard PFAS gradient methods utilize aqueous and organic mobile phases that contain an additive, typically ammonium acetate, that remains at a consistent pH throughout the gradient. This is appropriate for reverse phase columns that retain compounds based solely on their hydrophobicity or polarity and utilize increased organic concentration over the gradient to separate compounds. In the case of a mixed mode column like the

Atlantis Premier BEH C_{18} AX Column, the anion exchange selectivity is utilized by varying pH over the gradient which essentially activates (retention) and deactivates (elution) the ion exchange sites on the column. Therefore, the best resolving power is gained when both organic composition and pH are varied over the gradient. An example of this can be seen in Figure 2 which compares the chromatographic resolution of a selection of 44 PFAS on the Atlantis Premier BEH C_{18} AX Column using a typical water/methanol with ammonium acetate gradient at a constant pH (Figure 2A) to the resolution using a water/methanol with ammonium hydroxide gradient (Figure 2B) that increases pH over the gradient run. In the ammonium acetate gradient, all 44 PFAS elute within an approximate 3-minute window. Utilizing ammonium hydroxide as a mobile phase additive to create a pH gradient increases the resolution over an elution window of approximately 13 minutes. Benefits from the increased chromatographic resolution include increased mass spectral data quality by allowing more dwell time for each MRM function, as well as decreased chances of matrix interference from co-eluting matrix compounds.

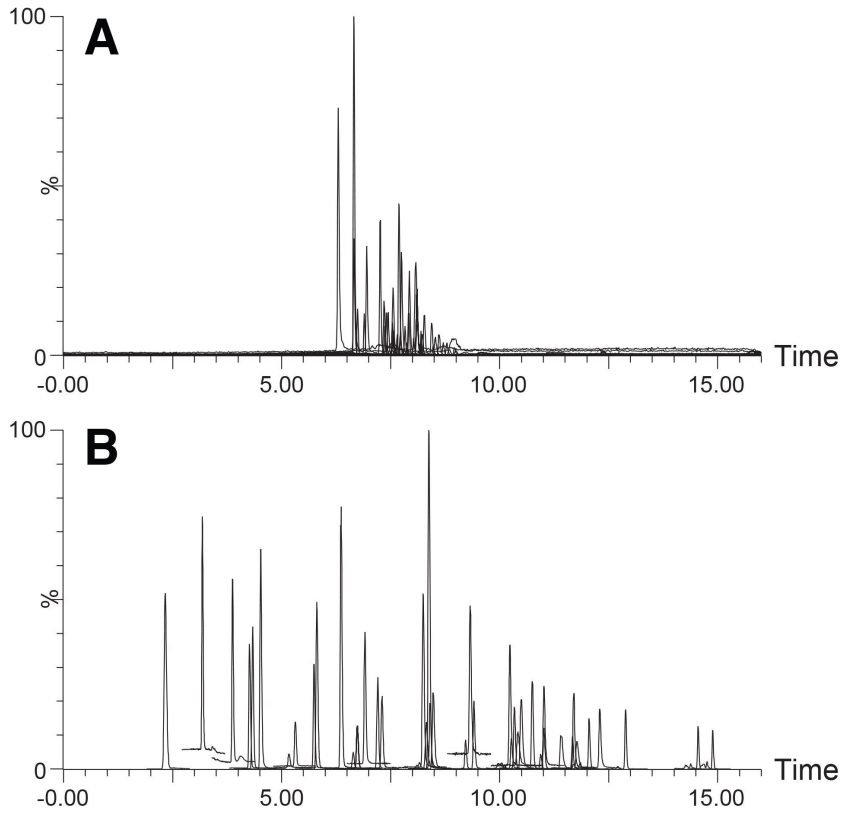

Figure 2. Comparison of the retention of 46 PFAS on the Atlantis Premier BEH C_{18} AX Column using a standard ammonium acetate gradient at constant pH (A) and the ammonium hydroxide gradient with varying pH (B).

Data quality guidelines required by ASTM 8421 were achieved upon final sample analysis on the mixed mode column in all samples, except for a few detections of TFA, PFPrA, and PFBA in the blank samples that are a result of solvent contamination. An overview in Figure 3 demonstrates the data quality guidelines were achieved during sample analysis of a wide range of sample types.

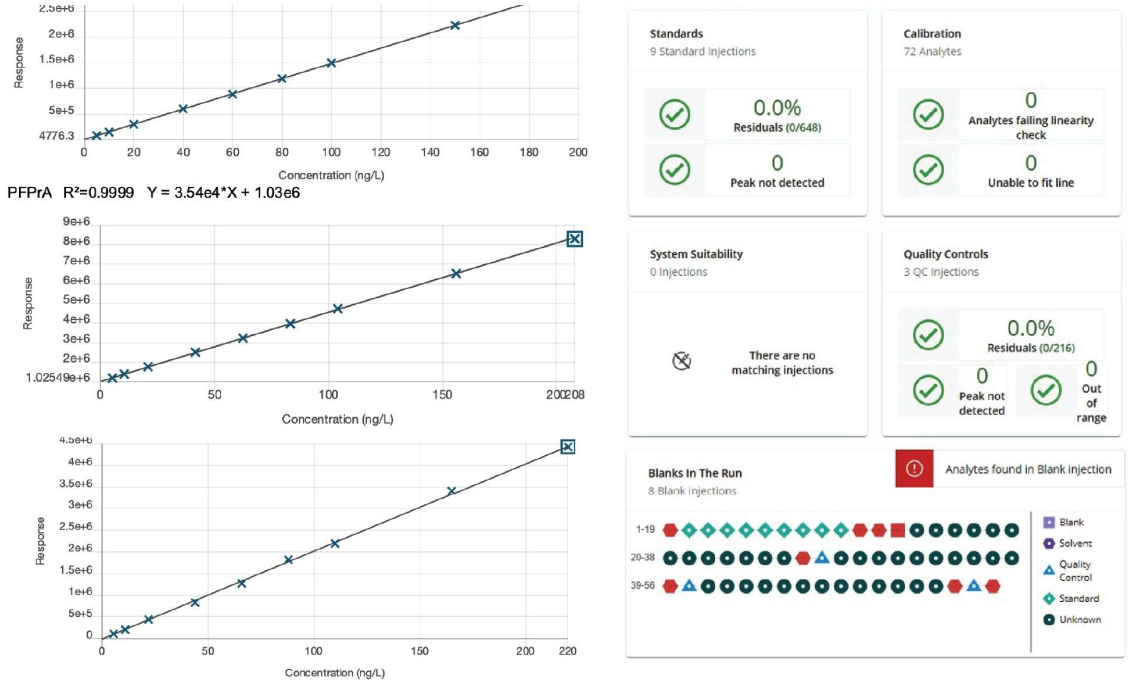

Figure 3. (Left) Calibration curves for 13C$_2$-TFA, PFPrA, and PFPrS over the range of 5–200 ng/L. TFA is represented using an isotope labelled analog of TFA due to contamination issues with the native TFA analog. (Right) waters_connect for quantitation overview page highlighting important ASTM data quality guidelines such as residuals, calibration, quality controls, and blanks.

During initial injections of the samples, the earliest eluting compounds did experience some severe retention time shifting that did not fall within the 5% expected retention time tolerance, as demonstrated in the top chromatogram of Figure 4. Once the retention time shift was observed in the early eluting compounds, the pH of the samples was tested. Even though an initial 10 µL acetic acid was added to each sample after dilution and filtration, as called for in the ASTM 8421 method, there were still a few samples that had elevated pH values. The solution used to create the calibration curve samples was approximately pH 4. Most of the samples analyzed did fall around pH 4 level with the 10 µL acetic acid added. However, the metal finisher sample tested at pH 5.5, the leachate tested near pH 5, and the pulp and paper sample tested at pH 4.5. It can be observed in Figure 4, that these three samples had reduced retention in accordance with their pH. The highest pH sample (water from the metal finisher) had the least retention (or earliest retention time) followed by the landfill leachate water, and then the pulp and paper factory water. Knowing this, additional acetic acid was added to each sample to adjust the pH

to 4 and the samples were re-analyzed. With all samples adjusted to the same nominal pH value, the bottom chromatogram of Figure 4 demonstrates the retention times of the early eluting compounds are much more stable and fall within the 5% retention time tolerance. Additionally, compounds throughout the rest of the gradient are stable and well within the 5% retention time tolerance (Figure 5). This highlights the importance of monitoring the pH of the final samples prior to injection on the mixed mode column. The sample pH may not prove to be as variable when preparing samples using SPE as this sample preparation technique should remove most of the matrix that may cause pH changes and the final samples should be more uniform.

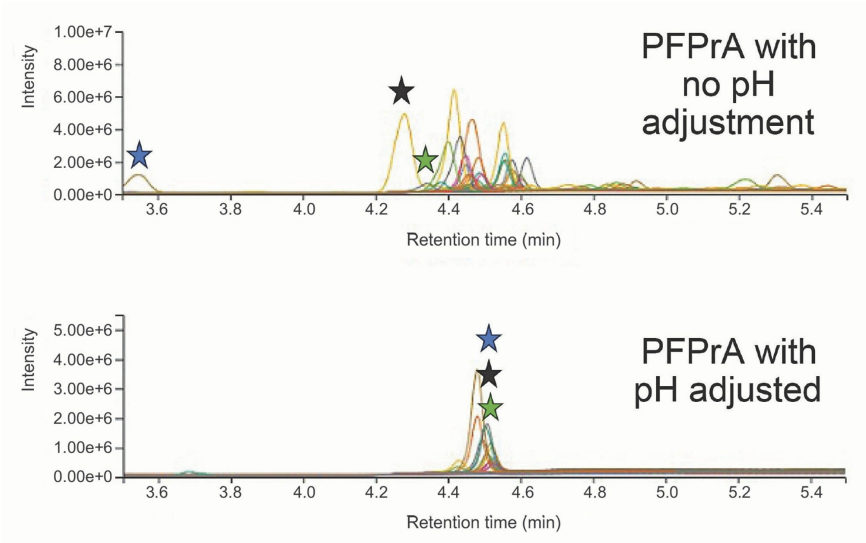

Figure 4. Overlap of PFPrA retention in different types of samples without (top) and with (bottom) additional pH adjustment. Stars indicate peaks from metal finisher (blue), leachate (black), and pulp and paper sample (green).

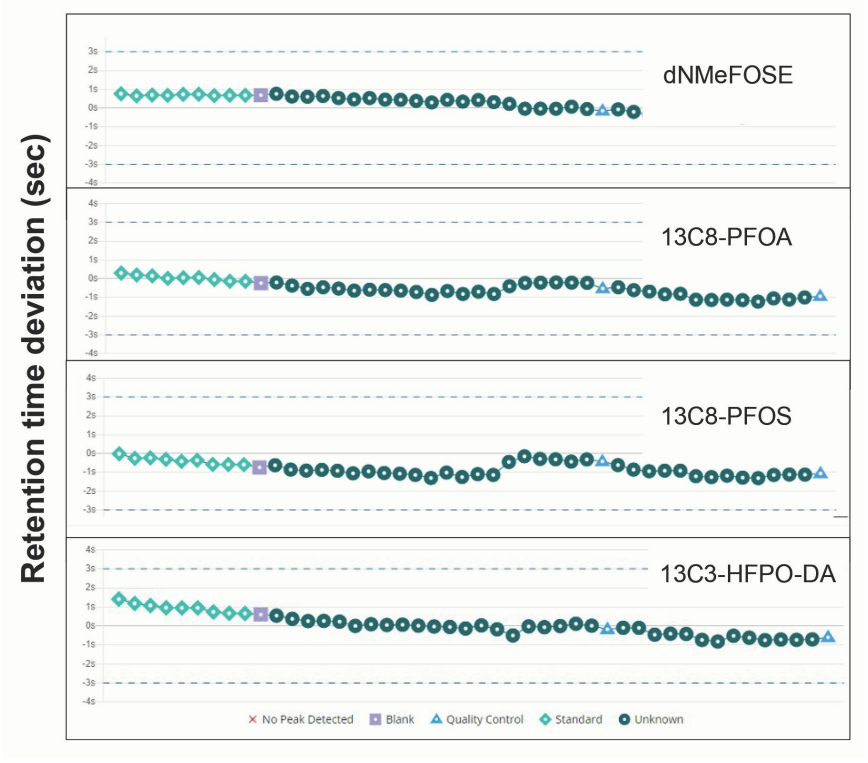

Figure 5. Retention time stability of different classes of PFAS on the Atlantis Premier BEH C_{18} AX Column.

In addition to ensuring the data fell within the quality control guidelines of the ASTM 8421 method, a certified reference material was analyzed and quantified in the same batch as the water samples. The results from this analysis can be observed in Figure 6 which also compares the quantified results from a reverse phase column. The mixed mode and reverse phase data are extremely comparable indicating that there are no major matrix components that co-elute using the C_{18} AX Column and causing ion suppression or enhancement. Most compounds quantified within the certified range of the standard, with a few quantifying slightly higher on both columns. This can potentially be explained by the fact that the certified values are based on a sample size of 500 mL and the sample size was adjusted to 5 mL for this study to replicate the sample size of the collected water samples. Therefore, the certified range may not be as accurate for this smaller sample size. Overall, the analysis of the wastewater CRM showed the mixed mode column analysis method to be accurate. Additionally, the mixed mode column analysis proved to be as accurate as the C_{18} reverse phase only column.

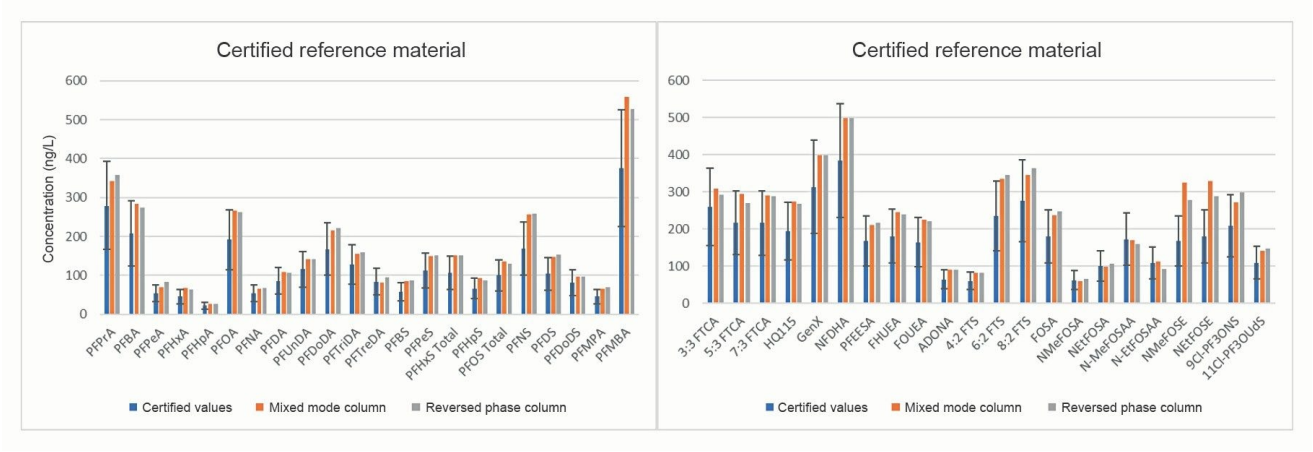

Figure 6. Performance of the method against an ERA certified reference material comparing the results obtained running on both the mixed mode column and reverse phase column.

Upon analysis of the different sample types on the Atlantis Premier BEH C_{18} AX Column, significant levels of TFA, PFPrA, and PFPrS were identified in the landfill leachate sample. Previous analysis of the samples using a reverse phase column (ACQUITY BEH C_{18} Column) only included PFPrA, which was poorly retained on the column. Without the inclusion of the ultra-short chain PFAS, made possible by the mixed mode chemistry of the Atlantis Premier BEH C_{18} AX Column, significant amounts of PFAS would have been missed in the analysis of this sample. Not only were the ultra-short chain PFAS included using the mixed mode column, but the rest of the PFAS normally targeted in routine testing methods could also be analyzed on the same column, in the same single injection. Table 2 lists the quantified amount of each PFAS identified in the landfill leachate sample using both the reverse phase and mixed mode columns as well as the calculated percent difference. The percentage difference between both sets of quantified results was within 15% for all PFAS identified except for PFBA, which had a percent difference of 33%. The higher percent difference for PFBA is assumed to be a result of possible co-eluting peaks that were resolved using the C_{18} AX column, causing an over-estimation of PFBA in the landfill leachate sample on the C_{18} column, as highlighted in Figure 7. The peaks circled in the C_{18} AX chromatogram appear to cause peak broadening/slight peak tailing of PFBA in the reverse phase chromatogram.

Compound	C_{18} AX (ng/L)	Reverse phase (ng/L)	% Difference	Compound	C_{18} AX (ng/L)	Reverse phase (ng/L)	% Difference
TFA	7790	–	NA	PFMPA	10.6	9.8	8.2
PFPrA	1063.6	1204	11.7	PFMBA	3	2.8	7.1
PFBA	1904.8	2853.2	33.2	3:3 FTCA	183.8	210	12.5
PFPeA	3150.8	3351.4	6.0	5:3 FTCA	6343.8	6176.2	2.7
PFHxA	5004.4	5002.4	0.0	7:3 FTCA	151.4	147.4	2.7
PFHpA	743.2	682	9.0	GenX	4.2	4	5.0
PFOA	1431	1379	3.8	NFDHA	ND	ND	ND
PFNA	133	129.2	2.9	PFEESA	ND	ND	ND
PFDA	153.4	147.4	4.1	FHUEA	48.8	48.4	0.8
PFUnDA	ND	ND	ND	FOUEA	ND	ND	ND
PFDoDA	ND	ND	ND	ADONA	ND	ND	ND
PFTriDA	ND	ND	ND	4:2 FTS	42.2	40.4	4.5
PFTreDA	ND	ND	ND	6:2 FTS	6829.2	7012.2	2.6
PFPrS	552	–	NA	8:2 FTS	69.2	69.4	0.3
PFBS	4055.8	4293.4	5.5	FOSA	11	10	10.0
PFPeS	348	361	3.6	NMeFOSA	ND	ND	ND
PFHxS	1133.8	1158.4	2.1	NEtFOSA	ND	ND	ND
PFHpS	29.4	32.2	8.7	N-MeFOSAA	254.6	222.4	14.5
PFOS	452.8	454	0.3	N-EtFOSAA	76.4	71.4	7.0
PFNS	ND	ND	ND	NMeFOSE	ND	ND	ND
PFDS	ND	ND	ND	NEtFOSE	ND	ND	ND
PFDoDS	ND	ND	ND	9Cl-PF3ONS	ND	ND	ND
HQ115	689.6	639	7.9	11Cl-PF3OUdS	ND	ND	ND

Table 2. Quantitation of 46 PFAS compounds in a landfill leachate sample using both the Atlantis Premier BEH C_{18} AX mixed mode Column and ACQUITY BEH C_{18} reverse phase Column, indicating the percent difference between both sets of data. (ND) not detected, (NA) not applicable.

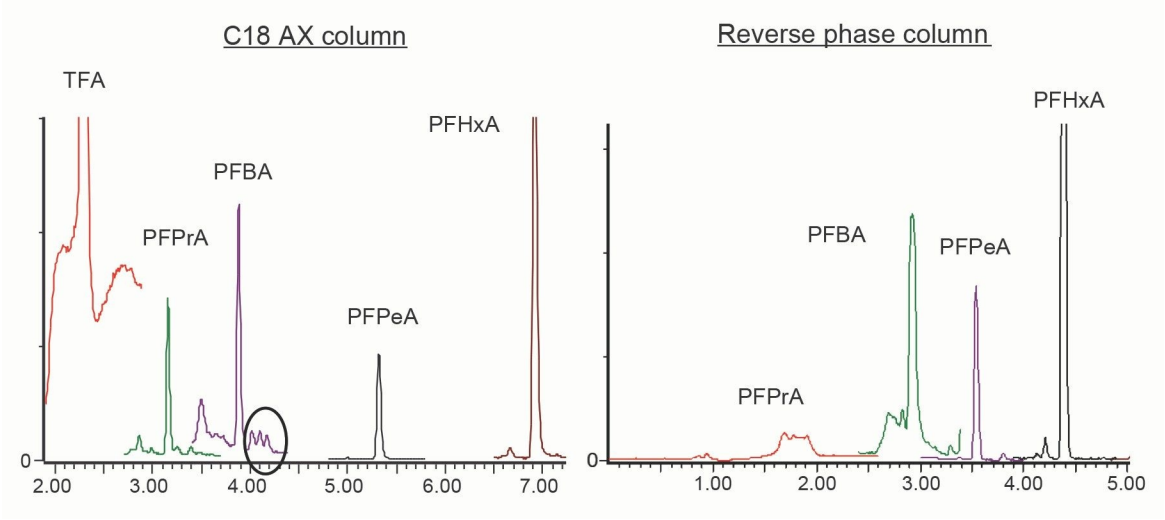

Figure 7. Zoomed in chromatogram of the landfill leachate sample showing the elution of C2–C6 carboxylates on the C_{18} AX and reverse phase columns. The co-eluting peaks that cause the higher PFBA quantitation on the reverse phase column and are resolved on the C_{18} AX column are circled. TFA and PFHxA peaks are cut off due to the zoom.

Conclusion

By taking advantage of the hydrophobic and ionic nature of PFAS, the Atlantis Premier BEH C_{18} AX Column was shown to successfully retain ultra-short chain PFAS, such as TFA and PFPrA, while maintaining the ability to analyze and quantify all other legacy, long chain PFAS in a single injection. A variety of water samples that differed quite drastically in composition were quantified according to the ASTM 8421 data quality guidelines. Results were also verified using an ERA certified wastewater reference material giving confidence to the use of the Atlantis Premier BEH C_{18} AX Column for a wide range of PFAS analysis. The use of the Atlantis Premier BEH C_{18} AX Column will allow laboratories to expand the suite of PFAS capable of analysis in a single injection from ultra-short chain through long chain PFAS on their current LC-MS/MS system.

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Appendix

Compound	Precursor	Fragment	CV	CE
TFA	112.9	68.9	8	10
PFPrA	162.9	118.9	10	10
PFBA	213.0	169	10	10
PFPeA	262.9	219	10	5
PFHxA	312.9	269	5	10
		119	5	20
PFHpA	362.9	319	15	10
		169	15	15
PFOA	412.9	369	10	10
		169	10	15
PFNA	462.9	419	10	10
		219	10	15
PFDA	512.9	468.9	15	9
		219	15	15
PFUnDA	562.9	518.9	25	10
		269	25	20
PFDoDA	612.9	568.9	30	10
		169	30	25
PFTriDA	662.9	618.9	5	10
		169	5	30
PFTreDA	712.9	668.9	10	25
		169	10	15
PFPrS	248.9	80.1	15	30
		99.1	15	30
PFBS	298.9	80.1	15	30
		99.1	15	30
PFPeS	348.9	79.9	10	30
		98.9	10	30
PFHxS	398.9	80.1	10	35
		99.1	10	30
PFHpS	448.9	80.1	15	35
		99.1	15	35
PFOS	498.9	80.1	15	40
		99.1	15	40
PFNS	548.9	80.1	20	40
		99.1	20	40
PFDS	598.9	80.1	46	46
		99.1	46	46
PFUnDS	649.1	80	40	55
		99	40	55
PFDoDS	699.1	80	40	55
		99	40	55
PFTrDS	749.1	80	40	55
		99	40	55
GenX (HFPO-DA)	285.0	169	5	7
		GenX	5	35
ADONA	376.9	251	10	10
		377.3	10	25
9Cl-PF3ONS	530.9	350.9	15	25
		82.9	15	25
11Cl-PF3OUdS	630.9	450.9	30	30
		631.2	30	30
HQ-115	279.9	146.9	5	25
		210.9	5	20
4:2 FTS	326.9	306.9	15	15
		327.3	15	35
6:2 FTS	426.9	407	10	20
		427.3	12	32
8:2 FTS	526.9	506.8	15	25
		527.3	15	37
3:3 FTCA	241.0	116.9	5	40
		176.9	5	10
5:3 FTCA	340.9	216.9	5	25
		237	5	10

Compound	Precursor	Fragment	CV	CE
7:3 FTCA	440.9	316.9	10	22
		337	10	17
PFEESA	314.9	82.9	15	20
		134.9	15	20
NFDHA	295.0	84.9	5	10
		200.9	5	10
FOUEA	456.9	393	20	11
FHUEA	356.9	292.9	20	12
FOSA	497.9	78	40	30
N-MeFOSA	511.9	168.9	40	30
		218.9	40	25
N-EtFOSA	525.9	168.9	5	25
		218.9	5	25
N-MeFOSE	616.0	59	15	15
N-EtFOSE	630.0	59	15	15
N-MeFOSAA	569.9	418.9	35	25
		219.1	35	20
N-EtFOSAA	584.0	418.9	15	20
		525.9	15	20
$^{13}C_2$-TFA	114.9	69.9	8	10
$^{13}C_3$-PFPrA	165.9	120.9	10	10
$^{13}C_3$-PFBA	216.9	172	10	10
$^{13}C_5$-PFPeA	267.9	223	10	5
$^{13}C_5$-PFHxA	317.9	272.9	10	5
		119.9	10	20
$^{13}C_4$-PFHpA	366.9	321.9	15	10
		169	15	15
$^{13}C_8$-PFOA	420.9	375.9	5	15
		172	5	10
$^{13}C_9$-PFNA	471.9	426.9	10	10
		223	10	15
$^{13}C_6$-PFDA	519	473.9	5	10
		219	5	15
$^{13}C_7$-PFUnDA	569.9	524.9	5	10
		274	5	15
^{13}C-PFDoDA	614.9	569.9	10	10
		169	10	25
$^{13}C_2$-PFTreDA	714.9	169	25	35
		669.9	25	10
$^{13}C_3$-PFBS	301.9	80.1	10	30
		99.1	10	25
$^{13}C_3$-PFHxS	401.9	80.1	10	40
		99.1	10	35
$^{13}C_8$-PFOS	506.9	80.1	15	40
		99.1	15	40
$^{13}C_8$-FOSA	505.9	78.1	35	25
d NMeFOSA	514.9	168.9	40	30
d NEtFOSA	531	168.9	5	25
d7-NMeFOSE	623	58.9	15	15
d9-NEtFOSE	639	58.9	15	15
D_5-N-EtFOSAA	589	418.9	30	20
		506.9	30	15
D_3-N-MeFOSAA	572.9	418.9	35	20
		482.7	35	15
$^{13}C_2$-4:2 FTS	328.9	308.9	40	15
		81	40	25
$^{13}C_2$-6:2 FTS	428.9	409	10	20
		80.9	10	27
$^{13}C_2$-8:2 FTS	528.9	508.9	10	20
		81	10	35
$^{13}C_3$-GenX	287	169	5	12
		119	5	12

Appendix Table 1. MS Method conditions for PFAS included in analysis.

Featured Products

ACQUITY UPLC I-Class PLUS System <https://www.waters.com/134613317>

waters_connect for Quantitation <https://www.waters.com/nextgen/global/products/informatics-and-software/waters_connect-for-quantitation.html>

Xevo TQ Absolute Triple Quadrupole Mass Spectrometry < https://www.waters.com/nextgen/global/products/mass-spectrometry-systems/xevo-tq-absolute.html>

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