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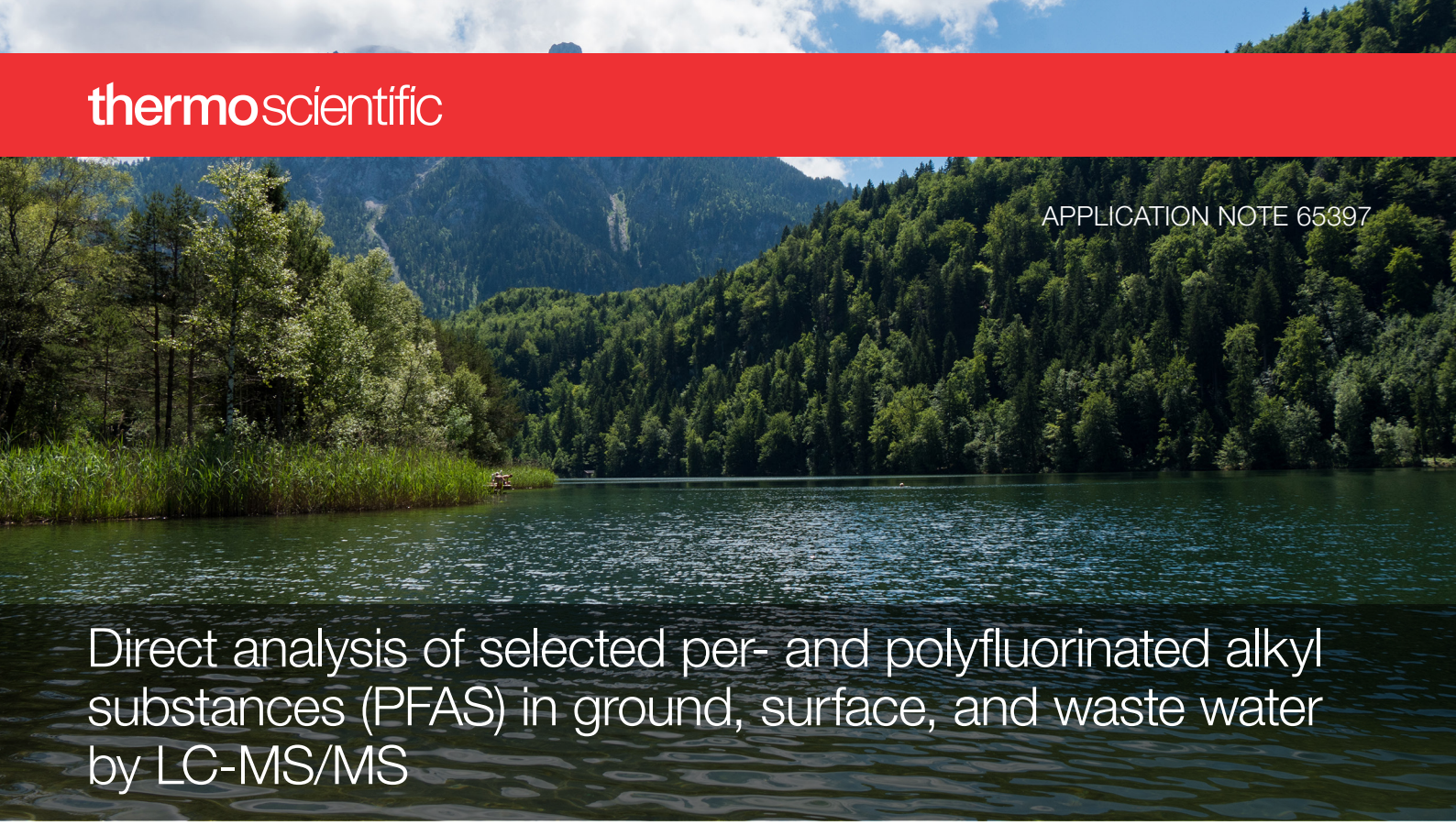

APPLICATION NOTE 65397

Direct analysis of selected per- and polyfluorinated alkyl substances (PFAS) in ground, surface, and waste water by LC-MS/MS

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Keywords

Perfluorinated organic compounds, PFAA, PFOS, PFOA, GenX, PFCs, environmental contaminants, emerging contaminants, EPA 8327, EPA 537, EPA 537.1

Goal

To demonstrate method performance for the PFAS analysis at low levels (ng/L) in a wide variety of non-drinking water matrices by direct analysis and submit data package for EPA 8327 interlaboratory method validation.

Introduction

Per- and polyfluoroalkyl substances (PFAS) are a group of man-made chemicals that includes perfluorooctanoic (PFOA), perfluorooctyl sulfonic acid (PFOS), and hexafluoropropylene oxide dimer acid (HFPO-DA, which is part of GenX process). PFAS compounds have been manufactured since the 1940s. The most well-known PFAS compounds, PFOA and PFOS, have been the most extensively produced and studied for chemical properties and toxicological effects. Both chemicals are very persistent in the environment and accumulate in the human body over time. It is well documented that exposure to PFAS can lead to adverse human health effects[1-3] and are found in food packaging material as well as food processing equipment. Plants can accumulate PFAS when grown in PFAS-containing soil and/or water. These compounds are also found in a wide variety of consumer products such as

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cookware, food containers (e.g., pizza boxes), and stain repellants. Additional products that lead to routes of exposure include clothing with stain- and water-repellent fabrics, nonstick products (e.g., Teflon), polishes, waxes, paints, and cleaning products. Another major source of PFAS are fire-fighting foams, which are a primary component of groundwater contamination at airports and military bases. More exposure comes from workplace environments, including production facilities or industries (e.g., chrome plating, electronics and manufacturing, or oil recovery).

Of particular note, drinking water can contain PFAS and can be associated with domestic and specific workplace facilities. Living organisms, including fish, animals and humans, have been shown to have accumulations of PFAS compounds and thus can build up and persist over time.[1-4] For these reasons, most people have been exposed to PFAS.

There is documented evidence that exposure to PFAS can lead to adverse health outcomes in humans.[3,4] Many studies indicate that PFOA and PFOS can cause reproductive and developmental, liver and kidney, and immunological effects in laboratory animals. Both chemicals have been found to cause tumors in animals. The most consistent findings are increased cholesterol levels among exposed populations, with more limited findings related to the following:

- low infant birth weights
- effects on the immune system
- cancer (for PFOA)
- thyroid hormone disruption (for PFOS)

PFAS compounds can be per- and polyfluorinated along a carbon backbone, typically ending with a carboxylic or sulfonic acid. PFOA and PFOS are made up of a C_8F_{17} subunit with either a carboxylic group (PFOA) or sulfonate group (PFOS). Replacement chemicals, like GenX, tend to have fewer carbon atoms in the chain, but have many similar physical and chemical properties as their predecessors (e.g., they both repel oil and water). Industries in the United States have phased out production of PFOA and PFOS because of health risks to humans and have been using replacement PFAS, such as GenX. There is a substantial body of knowledge for managing risk from PFOS and PFOA, but much less knowledge about the replacement PFAS.

The US EPA office of Ground Water and Drinking Water has developed a method specifically for the analysis of PFAS in drinking water, EPA 537, which is based on solid-phase extraction (SPE) followed by LC-MS/MS detection.[5] This methodology was developed for use during the EPA's Unregulated Contaminant Rule 3 (UCMR3) monitoring program.[6] Recently, an updated version of this method EPA 537.1 has been validated to include additional PFAS compounds such as GenX.[8] An alternative method developed for additional water matrices such as surface, ground, and waste waters is ASTM D7979,[7] and is based on simple sample extraction and filtration followed by LC-MS/MS analysis. This application note describes a direct analysis method for the determination of a list of 24 PFAS in a wide variety of non-drinking water matrices. The data was used for the validation of a new method, EPA 8327, for a wide variety of water matrices as part of an interlaboratory study sponsored by the EPA Office of Water.

Experimental

This application note describes the quantitation of selected PFAS in reagent, ground, surface, and waste water based on the recent EPA 8327 method. The list of PFAS included in this study is shown in Table 1.

LC-MS/MS analysis

Since the required limits of detection are in the low ng/L range, careful selection of reagents and consumables is necessary to ensure they are PFAS-free. Therefore, the LC-MS/MS system comprised a Thermo Scientific™ Vanquish™ Flex Binary UHPLC system fitted with a Thermo Scientific™ PFC-free kit (P/N 80100-62142) and interfaced with a Thermo Scientific™ TSQ Altis™ triple quadrupole mass spectrometer equipped with a HESI ionization probe. An isolator column was also installed after the LC pump and prior to the injection valve to offset background contaminants from the LC pump, autosampler, degasser, and mobile phases.

Table 1. List of PFAS compounds included in this method

Analytes	Abbreviation	CAS number	Surrogates
PFAS Sulfonic Acids			
Perfluorobutyl sulfonic acid	PFBS	29420-49-3	$^{13}C_3$-PFBS
Perfluorohexyl sulfonic acid	PFHxS	3871-99-6	$^{13}C_3$-PFxS
Perfluorooctyl sulfonic acid	PFOS	1763-23-1	$^{13}C_8$-PFOS
1H, 1H, 2H, 2H-perfluorohexane sulfonic acid	4:2 FTS	757124-72-4	$^{13}C_2$-4:2 FTS
1H, 1H, 2H, 2H-perfluorooctane sulfonic acid	6:2 FTS	27619-97-2	$^{13}C_2$-6:2 FTS
1H, 1H, 2H, 2H-perfluorodecane sulfonic acid	8:2 FTS	39108-34-4	$^{13}C_2$-8:2 FTS
Perfluoro-1-pentanesulfonic acid	PFPeS	706-91-4	-
Perfluoro-1-heptanesulfonic acid	PFHpS	375-92-8	-
Perfluoro-1-nonanesulfonic acid	PFNS	68259-12-1	-
Perfluoro-1-decanesulfonic acid	PFDS	2806-15-7	-
PFAS Carboxylic Acids			
Perfluorobutanoic acid	PFBA	375-22-4	$^{13}C_4$-PFBA
Perfluoropentanoic acid	PFPeA	2706-90-3	$^{13}C_5$-PFPeA
Perfluorohexanoic acid	PFHxA	307-24-4	$^{13}C_5$-PFHxA
Perfluoroheptanoic acid	PFHpA	375-85-9	$^{13}C_4$-PFHpA
Perfluorooctanoic acid	PFOA	335-67-1	$^{13}C_8$-PFOA
Perfluorononanoic acid	PFNA	375-95-1	$^{13}C_9$-PFNA
Perfluorodecanoic acid	PFDA	335-76-2	$^{13}C_6$-PFDA
Perfluoroundecanoic acid	PFUnA	2058-94-8	$^{13}C_7$-PFUnA
Perfluorododecanoic acid	PFDoA	307-55-1	$^{13}C_2$-PFDoA
Perfluorotridecanoic acid	PFTriA	72629-94-8	-
Perfluorotetradecanoic acid	PFTreA	376-06-7	$^{13}C_2$-PFTreA
PFAS sulfonamides and sulfonamidoacetic acids			
N-ethylperfluoro-1-octanesulfonamidoacetic acid	N-EtFOSAA	2991-50-6	D_3-N-EtFOSAA
N-methylperfluoro-1-octanesulfonamidoacetic acid	N-MeFOSAA	2355-31-9	D_3-N-MeFOSAA
Perfluoro-1-octanesulfonamide	PFOSA	754-91-6	$^{13}C_8$-PFOSA

LC conditions	
Analytical column:	Thermo Scientific™ Accucore™ RP-MS, 2.6 µm, 2.1 × 100 mm (P/N 17626-102130)
Isolator column:	Thermo Scientific™ Hypersil™ BDS C18, 5 µm, 2.1 × 50 mm (P/N 28105-052130)
Column temp.:	45 °C
Flow rate:	0.5 mL/min
Solvent A:	Water containing 2 mM ammonium acetate, 2% methanol, and 0.1% acetic acid
Solvent B:	Methanol containing 2 mM ammonium acetate, 2% water, and 0.1% acetic acid

LC conditions (continued)		
Injection volume:	25 µL	
Gradient:	Time (min)	% Solvent B
	0	0
	1	30
	6	45
	13	80
	14	95
	17	95
	18	0
	21	0

Optimized MS parameters	
HESI source:	Negative ionization mode
Spray voltage:	2.5 kV
Sheath gas:	50 arb
Auxiliary gas:	10 arb
Ion transfer tube temp.:	325 °C
Vaporizer temperature:	300 °C

Optimized MS parameters (continued)	
Cycle time for the negative SRM transitions:	0.3 s
Q1 resolution:	0.7 Da
Q3 resolution:	1.2 Da
CID gas:	2 mTorr

Table 2 summarizes the monitored SRM transitions.

Table 2 (part 1). Monitored SRM transitions details

Compound	Retention time (min)	Precursor (*m/z*)	Product (*m/z*)	Collision energy (V)	RF lens (V)
PFBA	2.70	212.979	168.97	9	30
$^{13}C_4$-PFBA	2.70	216.993	172	9	30
PFPeA	4.98	262.976	219.042	9	31
$^{13}C_5$-PFPeA	4.98	267.993	222.99	9	32
PFBS	5.73	298.943	79.957	34	116
		298.943	98.956	29	116
$^{13}C_3$-PFBS	5.73	301.953	79.96	34	119
PFHxA	7.94	312.973	119.042	18.76	39
			268.97	9	39
$^{13}C_5$-PFHxA	7.94	317.99	273	9	37
4:2 FTS	7.66	326.974	81.042	26.07	115
			286.958	23	115
			307.042	18.11	115
$^{13}C_2$-4:2 FTS	7.66	328.981	308.96	18	103
PFPeS	8.42	348.94	80.042	33.66	145
			99	31	145
			119.054	31.42	145
PFHpA	9.91	362.97	119.054	19.52	43
			168.97	15.53	43
			319.042	9	43
$^{13}C_4$-PFHpA	9.91	366.983	321.98	9	43
PFHxS	10.11	398.937	79.957	39	135
			98.956	35	135
$^{13}C_3$-PFxS	10.11	401.947	79.957	39	133
PFOA	11.22	412.966	169	16.1	49
			219	14.55	49
			369.042	9	49
$^{13}C_8$-PFOA	11.22	420.993	376	9	48
6:2 FTS	11.12	426.968	81.042	29.94	123
			386.97	26.72	123
			406.988	21.45	123
$^{13}C_2$-6:2 FTS	11.12	428.975	408.96	21	123
PFHpS	11.30	448.933	80.012	37.6	131
			98.97	36.2	131
			169.03	31.04	131

Table 2 (part 2). Monitored SRM transitions details

Compound	Retention time (min)	Precursor (*m/z*)	Product (*m/z*)	Collision energy (V)	RF lens (V)
PFNA	12.21	462.963	169	17.51	52
			219.012	15.23	52
			418.97	9	52
$^{13}C_9$-PFNA	12.21	471.993	426.97	9	52
PFOS	12.24	498.93	79.957	47	159
			98.956	40	159
$^{13}C_8$-PFOS	12.24	506.957	79.957	40	160
PFDA	11.58	512.96	219.012	16.14	56
			269.042	15.8	56
			469.042	9	56
$^{13}C_6$-PFDA	11.58	518.98	473.97	9	56
8:2 FTS	13	526.962	81.012	34.83	137
			487	28.92	137
			506.97	24.37	137
$^{13}C_2$-8:2FTS	13	528.968	508.96	24	137
PFNS	13.04	548.927	80.071	42.34	148
			98.97	40.67	148
			229.958	41.66	148
PFUdA	13.73	562.957	219	17.32	62
			269.03	16.94	62
			518.97	9	62
NMeFOSAA	13.64	569.967	418.97	18.42	107
			512	19.55	107
$^{13}C_7$-PFUnA	13.73	569.98	524.97	9	62
d_3-N-MeFOSAA	13.64	572.986	418.97	18	107
PFOSA	13.66	497.946	78.071	29.37	127
			169.03	25.85	127
			478.042	22.51	127
$^{13}C_8$-PFOSA	13.66	505.973	77.97	29	127
NEtFOSAA	14.04	583.983	418.97	18.34	101
			482.958	13.9	101
			526.03	18.26	101
d_5-N-EtFOSAA	14.04	589.014	418.97	18	101
PFDS	13.70	598.924	80.042	44.92	169
			98.929	43.48	169
			229.929	46.09	169
PFDoA	14.30	612.954	169.03	23.69	67
			319.042	17.54	67
			569	9	67
$^{13}C_2$-PFDoA	14.30	614.96	569.97	9	67
PFTriA	14.63	662.95	168.97	25.16	71
			369.071	17.85	71
			619.042	9	71
PFTreA	14.83	712.947	319.054	19.86	74
			369.042	18.87	74
			668.97	9	74
$^{13}C_2$-PFTreA	14.83	714.954	669.96	9	74

Data processing

Thermo Scientific™ Chromeleon™ Chromatography Data System software, version 7.2.9

All materials were demonstrated to be free from interferences by analyzing method blanks. All glassware, including syringes and filters, were thoroughly cleaned with methanol prior to sample preparation. All solvents used in sample preparation, standards preparation, and chromatography were Thermo Scientific UHPLC-MS grade.

Sample preparation

PFAS standard solutions

Target and surrogate PFAS standard mixtures in methanol at 2000 and 1000 µg/L, respectively, were purchased from Wellington Laboratories and kept away from PFAS packaging and material during storage. A stock solution of 24 target PFAS compounds was prepared in methanol at a concentration of 2 µg/L. Calibration solutions, with concentrations of 5–200 ng/L (ppt), were prepared by serial dilutions of the stock solution in 50:50 (v/v) methanol/water containing 0.1% acetic acid.

Non-drinking water matrices

Field water samples (5 mL) were provided by the US EPA Region 5 and included reagent water, surface water, ground water, and waste water through a participating EPA study. Each water sample was spiked with a low (60 ng/L) and high level (200 ng/L) of a selected target PFAS compounds (five replicates of each) prior to shipment to the lab. Five blank samples of each water matrix were also provided.

The 5 mL water samples were then spiked with 40 µL of a 20 µg/L isotopically labeled PFAS surrogates solution (Table 1). 5 mL of methanol were added and the mixture vortexed for 1 minute. The mixture was then filtered through a washed Acrodisc® GxF/0.2 µm GHP membrane syringe-driven filter with methanol and acetonitrile (Pall Corporation, P/N AP-4305). The 10 mL filtrates were acidified by addition of 10 µL of acetic acid, and an aliquot of each sample was transferred to a polypropylene autosampler vial (Thermo Fisher Scientific, P/N C4013-13) sealed with a polyethylene cap with integrated polyethylene membrane (P/N C4013-50Y).

Control samples

The EPA 8237 method requires control samples (method blank, laboratory control, and reporting limit checking samples) to be run with field non-drinking water samples. Therefore, two method blanks were prepared by measuring 5 mL of water UHPLC-MS grade into 15 mL polypropylene Falcon™ tubes (BD Falcon, P/N 14-959-70C) and spiking with 40 µL of a 20 µg/L PFAS surrogate solution in methanol. Two laboratory control samples were prepared by spiking 5 mL of water UHPLC-MS grade at 160 ng/L of 24 selected PFAS, and a reporting limit of quantitation checking sample was prepared by spiking 5 mL of water UHPLC-MS grade at 10 ng/L. Control samples were then taken through the sample preparation as field water samples.

Results and discussion

Excellent chromatographic separation was achieved on an Accucore RP-MS analytical column using different mobile phases compositions. Figure 1 shows an overlaid chromatogram of all PFAS compounds analyzed in this method.

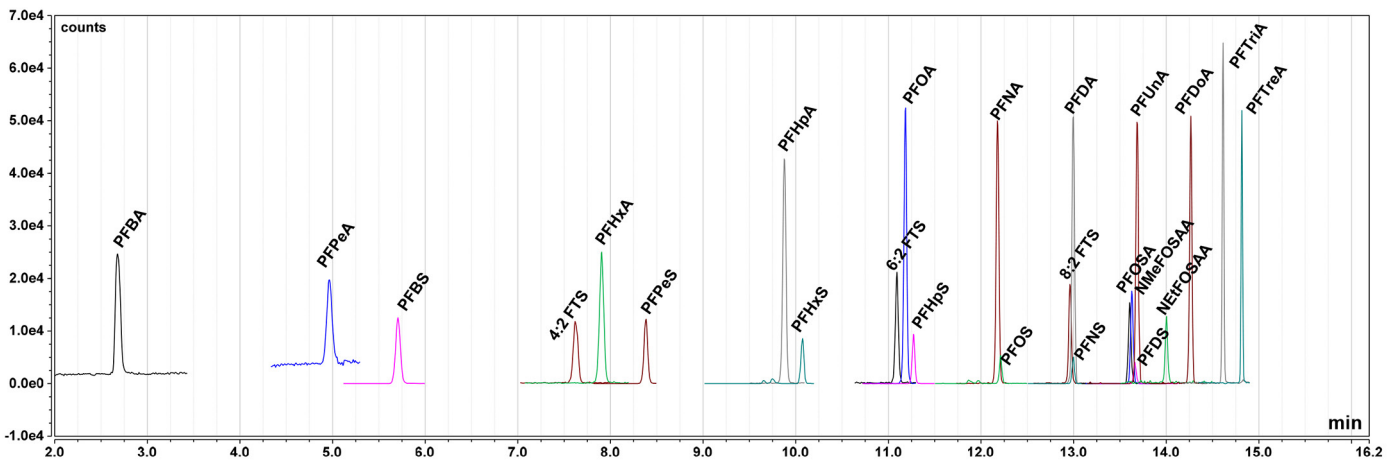

Figure 1. Overlaid chromatograms of all PFAS compounds included in this method

Linearity and sensitivity

Excellent linearity and quantitative accuracy were achieved over the range of 5 to 200 ng/L, with correlation coefficients greater than 0.99 for all transitions and the respective residuals within 20% of the nominal values. Representative calibration curves for PFOS and PFTriA are shown in Figure 2, with correlation coefficients of 0.9955 and 0.9950, respectively. Figure 2 also shows chromatograms of overlaid quantitation and confirming ions injected at 1 ng/L, which is five times lower than the LLOQ reported by ASTM D7979-17 for these two compounds. Additionally, Table 3 shows the LLOQs for all 24 PFAS analyzed in this method, based on accuracy and RSD ≤20%, demonstrating the high sensitivity achieved with the TSQ Altis mass spectrometer for the quantitation of PFAS at very low levels (ppt range).

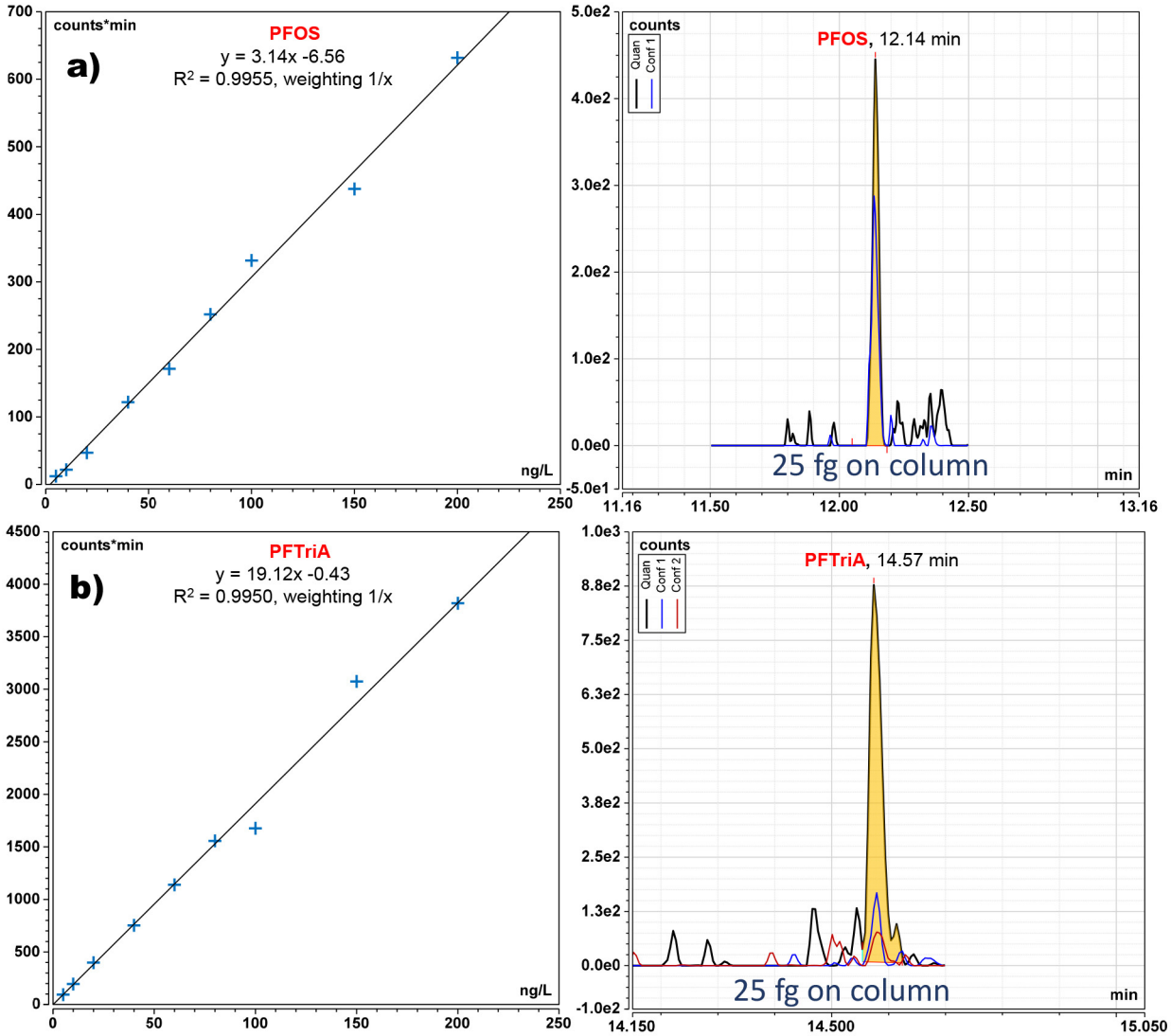

Figure 2. Representative calibration curves for a) PFOS and b) PFTriA, and chromatograms of an injection of 1 ng/L, which is five times lower than the reporting limit of quantitation

Table 3. Reporting lower limit of quantitation obtained by this method and ASTM D7979-17 reporting ranges

Compound	LLOQ* (N=3) (ng/L)	ASTM D7979-17 reporting ranges* (ng/L)
PFBA	10	50–2000
PFPeA	10	50–2000
PFBS	2	10–400
4:2 FTS	10	-
PFHxA	2	10–400
PFPeS	2	-
PFHpA	5	10–400
PFHxS	5	10–400
6:2 FTS	5	-
PFOA	2	10–400
PFHpS	2	-
PFNA	2	10–400
PFOS	2	10–400
8:2 FTS	5	-
PFDA	2	10–400
PFNS	10	-
N-MeFOSAA	5	-
PFOSA	10	-
PFDS	10	-
PFUnA	2	10–400
N-EtFOSAA	5	-
PFDoA	2	10–400
PFTriA	2	10–400
PFTreA	2	10–400

*Concentrations taking into consideration the 50% dilution with methanol.

Control samples

Table 4 summarizes the method control criteria, and the results demonstrate all compounds passed in this method. Figure 3 shows the overlaid chromatogram of all PFAS of a method blank and a reagent water spiked at 10 ng/L (LLOQ checking sample) and taken through sample preparation. PFBA and PFPeA are quantifiable at an injected concentration of 5 ng/L, which is much lower than the reported limit of quantitation in EPA 8327 and ASTM D7979 (25 ng/L without considering 2-fold dilution in methanol).

Sample analysis

Each water matrix was spiked at low and high concentrations as described, (N=5 ea.) The 60 samples received were divided into three batches of 20 samples and analyzed on three different days. All 24 PFAS compounds were detected and quantifiable at both low and high spike concentrations. Figure 4 shows an example of overlaid chromatograms of all PFAS spiked at 60 ng/L in reagent, ground, surface, and waste samples. In Figure 4 fronting was observed with the first eluting chromatographic peaks in ground, surface, and waste water samples due to the overload of the analytical column by large injection volumes (25 µL). Reduced injection volumes (15 µL) improved peak shape and will also improve robustness (due to less matrix on column) while still maintaining good sensitivity as shown in Figure 5.

Table 4. Summary of method control criteria

Sample Type	Definition	Criteria	Results
Reagent blank	Methanol: Water (50:50, v/v) + 0.1% acetic acid	Concentration must be one half the LLOQ	Target compounds NOT DETECTED OR BELOW <LLOQ
Method blank	Reagent water + surrogates at 160 ng/L. Taken through sample preparation	Concentration must be one half the LLOQ	Target compounds NOT DETECTED OR BELOW LLOQ
LLOQ checking	Reagent water + targets at 10 ng/L. Taken through sample preparation	S/N ratio ≥3 for all quantitative ions & Target Recoveries <50% deviation	LLOQ at 10 ppt Recoveries <30% deviation for most of the compounds
Laboratory controls	Reagent water + targets at 160 ng/L. Taken through sample preparation.	Target recoveries <30% deviation	Target recoveries <30% deviation for most of the compounds

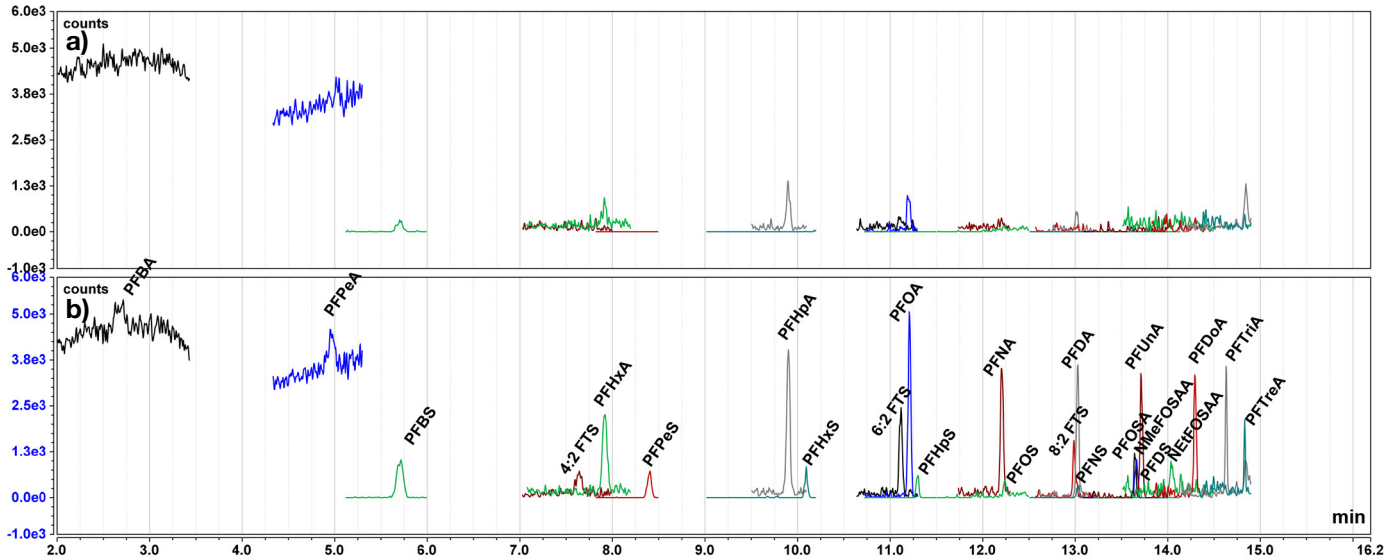

Figure 3. PFAS overlaid chromatograms: a) method blank sample and b) reporting limit checking sample spiked at 10 ng/L

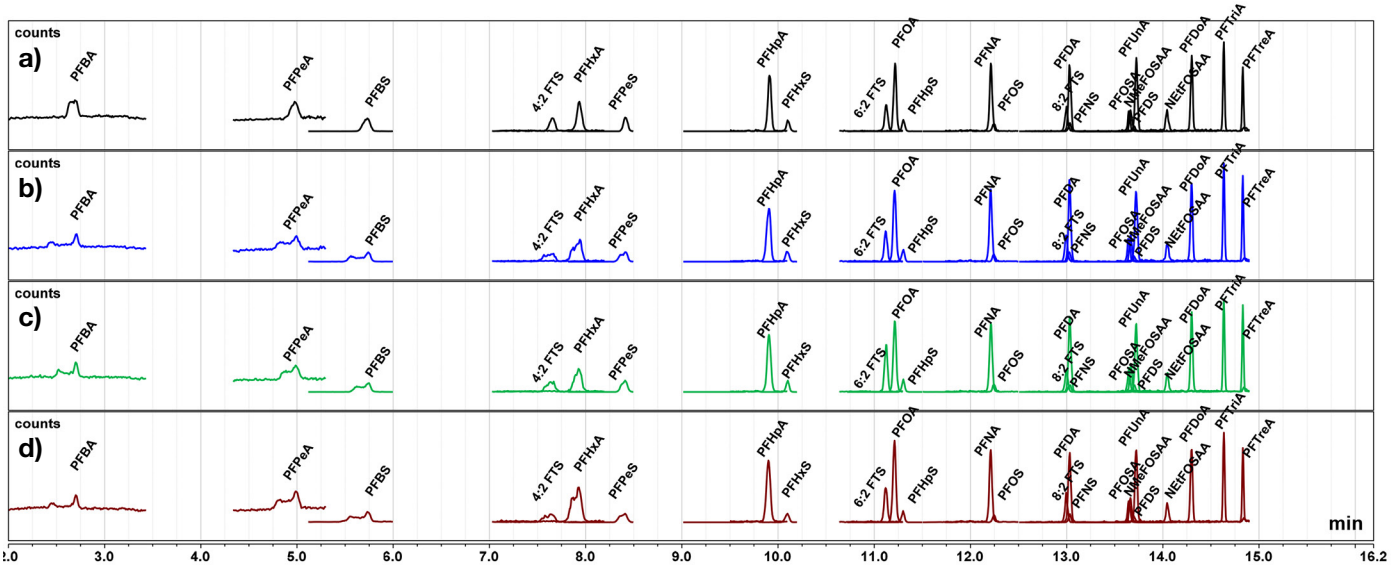

Figure 4. Overlaid chromatograms of 24 PFAS spiked at 60 ng/L in field samples: a) Reagent water; b) ground water; c) surface water; and d) waste water

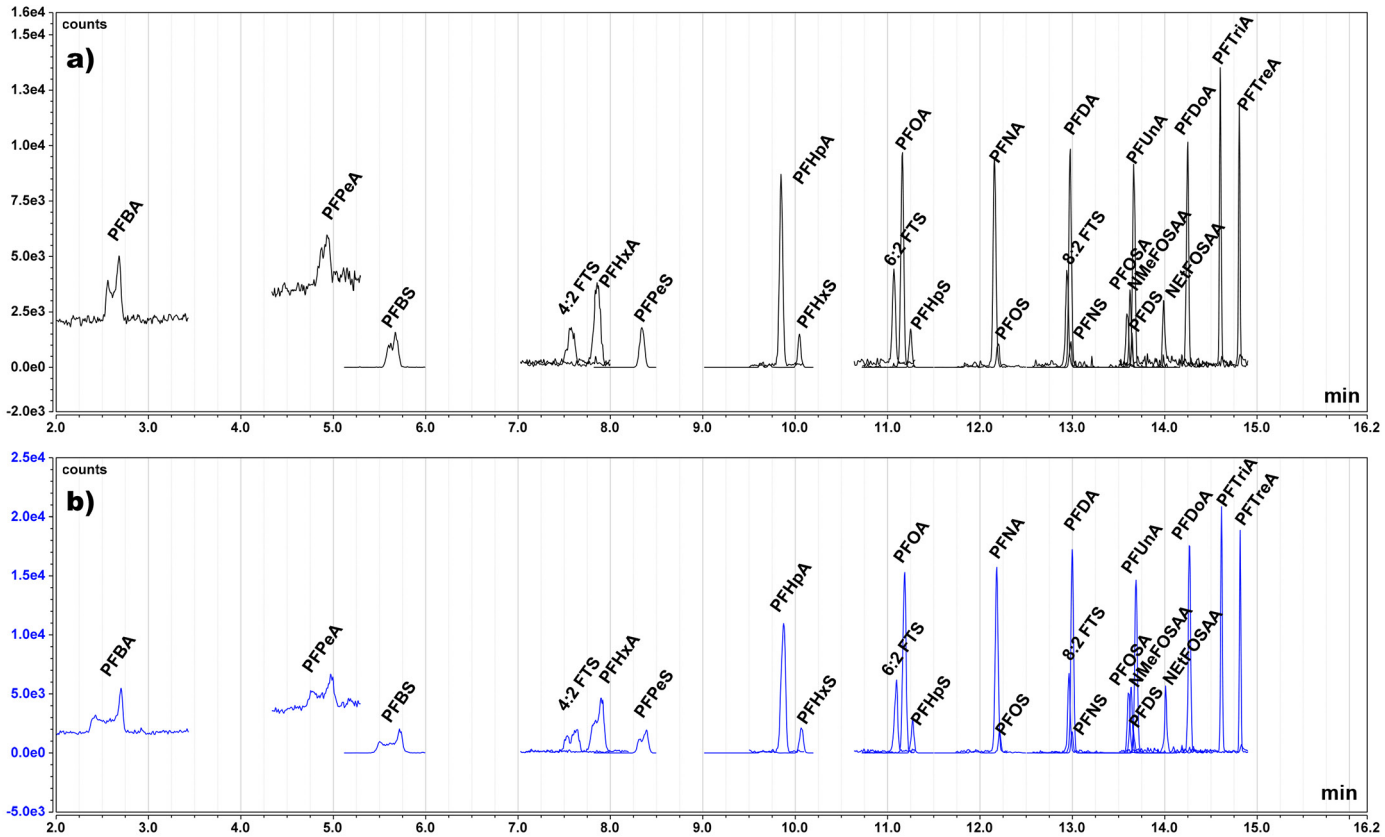

Figure 5. Overlaid chromatograms of a ground water sample spiked at 60 ng/L: a) 15 µL injection volume; b) 25 µL injection volume

Recovery of the 24 PFAS compounds spiked into the different water matrices is summarized in Table 5. All compounds analyzed in this method were within the range of 70% to 130% as required, except for PFBA spiked at low level in waste water (58% with an imprecision of 34%). The lower recovery observed may be related to co-eluting waste water matrix components causing signal suppression.

Table 5. PFAS recoveries in different water matrices, low and high levels at 60 and 200 ng/L, respectively

Compound	Recoveries %							
	Reagent water		Ground water		Surface water		Waste water	
	Low level	High level	Low level	High level	Low level	High level	Low level	High level
PFBA	77%	78%	71%	75%	74%	74%	58%	75%
PFPeA	84%	80%	104%	80%	115%	81%	88%	78%
PFBS	87%	81%	95%	81%	95%	79%	72%	77%
PFHxA	82%	81%	83%	79%	86%	80%	77%	74%
4:2 FTS	81%	82%	90%	78%	87%	79%	76%	91%
PFPeS	80%	80%	82%	79%	85%	78%	80%	83%
PFHpA	84%	81%	88%	80%	89%	80%	74%	81%
PFHxS	81%	81%	87%	78%	94%	81%	85%	85%
6:2 FTS	84%	82%	85%	80%	87%	94%	78%	79%
PFOA	83%	80%	88%	82%	123%	83%	83%	86%
PFHpS	81%	81%	84%	76%	83%	78%	79%	86%
PFNA	79%	81%	84%	80%	86%	80%	79%	82%
PFOS	91%	82%	91%	78%	93%	81%	79%	90%
8:2 FTS	85%	80%	81%	75%	76%	79%	78%	83%
PFNS	85%	75%	89%	79%	81%	76%	72%	78%
PFDA	80%	81%	86%	78%	85%	79%	74%	83%
NMeFOSAA	77%	81%	80%	77%	86%	81%	82%	84%
PFOSA	76%	76%	87%	75%	91%	75%	79%	81%
PFDS	82%	78%	89%	77%	85%	79%	72%	81%
PFUnA	76%	76%	80%	81%	75%	78%	75%	83%
NEtFOSAA	82%	79%	89%	77%	89%	81%	80%	85%
PFDoA	79%	82%	83%	78%	85%	82%	79%	85%
PFTriA	87%	86%	89%	79%	92%	91%	87%	89%
PFTreA	109%	103%	112%	91%	113%	119%	100%	110%

The LC-MS/MS method has proven to be very reproducible and robust as demonstrated by the precision values of all PFAS compounds spiked in non-drinking water matrices (N=5) summarized in Table 6.

Table 6. Reproducibility represented by % CV of 24 PFAS compounds analyzed in this method

Compound	Precision (CV, %)							
	Reagent water		Ground water		Surface water		Waste water	
	Low level	High level	Low level	High level	Low level	High level	Low level	High level
PFBA	6%	3%	23%	6%	17%	6%	34%	6%
PFPeA	9%	6%	9%	6%	25%	9%	9%	3%
PFBS	7%	4%	7%	4%	15%	3%	13%	3%
PFHxA	4%	4%	5%	3%	11%	4%	3%	10%
4:2 FTS	6%	1%	2%	4%	15%	7%	10%	18%
PFPeS	2%	4%	6%	4%	16%	3%	8%	4%
PFHpA	6%	3%	6%	5%	11%	3%	5%	3%
PFHxS	4%	5%	10%	6%	17%	4%	16%	5%
6:2 FTS	12%	4%	9%	4%	16%	14%	26%	7%
PFOA	4%	5%	8%	8%	32%	11%	12%	10%
PFHpS	12%	2%	6%	5%	14%	6%	10%	10%
PFNA	6%	4%	5%	3%	14%	3%	7%	3%
PFOS	13%	5%	5%	4%	13%	4%	5%	4%
8:2 FTS	6%	6%	11%	5%	16%	5%	8%	4%
PFNS	10%	6%	11%	4%	10%	3%	13%	5%
PFDA	4%	3%	6%	4%	19%	5%	5%	4%
NMeFOSAA	11%	7%	11%	5%	18%	4%	11%	3%
PFOSA	11%	10%	13%	5%	17%	8%	8%	5%
PFDS	10%	8%	3%	5%	13%	2%	4%	8%
PFUnA	9%	5%	3%	5%	25%	4%	8%	4%
NEtFOSAA	16%	4%	7%	5%	21%	8%	13%	5%
PFDoA	6%	5%	4%	6%	15%	8%	9%	4%
PFTriA	8%	5%	10%	6%	15%	11%	6%	5%
PFTreA	22%	14%	19%	12%	20%	23%	14%	14%

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Conclusions

The method referenced in this application note shows excellent quantitative performance of the TSQ Altis mass spectrometer for PFAS direct analysis in the low ng/L range in non-drinking water matrices.

- The Accucore RP-MS column provides excellent chromatographic separation and maintains robustness in challenging water matrices.
- The TSQ Altis mass spectrometer can quantitate the majority of PFAS compounds five times lower than the LLOQ reporting requirements in ASTM D7979-17 and EPA 8327 as demonstrated by the results shown in Table 3.
- PFAS compounds were detected in the different water matrices at both low and high spike concentrations with recoveries within the range required.
- All spiked water samples, in a variety of matrices, showed RSDs below 20% for most of the PFAS compounds, demonstrating the high robustness and reproducibility of the method.

References

1. National Institute of Environmental Health Sciences. Perfluorinated Chemicals (PFCs), https://www.niehs.nih.gov/health/materials/perflourinated_chemicals_508.pdf (Accessed November 27, 2018)
2. U.S. Environmental Protection Agency (EPA). Per- and Polyfluoroalkyl Substances (PFAS), https://www.epa.gov/pfas (Accessed November 27, 2018)
3. Agency for Toxic Substances and Disease Registry (ATSDR). An Overview of Perfluoroalkyl and Polyfluoroalkyl Substances and Interim Guidance for Clinicians Responding to Patient Exposure Concerns. https://www.atsdr.cdc.gov/pfc/docs/pfas_clinician_fact_sheet_508.pdf (Accessed November 29, 2018)
4. Stahl, T., Mattern, D., Brunn, H. Toxicology of perfluorinated compounds. *Environmental Sciences Europe* **2011,** *23,* 38. https://doi.org/10.1186/2190-4715-23-38
5. U.S Environmental Protection Agency (EPA). Method 537. Determination of Selected Perfluorinated Alkyl Acids in Drinking Water by Solid Phase Extraction and Liquid Chromatography/Tandem Mass Spectrometry (LC/MS/MS). https://nepis.epa.gov/Exe/ZyPDF.cgi?Dockey=P100EQ6W.txt (Accessed November 27, 2018)
6. U.S Environmental Protection Agency (EPA). Unregulated Contaminant Monitoring Rule 3 (UCMR3). https://www.epa.gov/dwucmr/third-unregulated-contaminant-monitoring-rule (Accessed November 27, 2018)
7. ASTM D7979-17, Standard Test Method for Determination of Per- and Polyfluoroalkyl Substances in Water, Sludge, Influent, Effluent and Wastewater by Liquid Chromatography Tandem Mass Spectrometry (LC/MS/MS), ASTM International, West Conshohocken, PA, 2017, www.astm.org (Accessed November 27, 2018)
8. U.S. Environmental Protection Agency (EPA). EPA 537.1 DETERMINATION OF SELECTED PERFLUORINATED ALKYL ACIDS IN DRINKING WATER BY SOLID PHASE EXTRACTION AND LIQUID CHROMATOGRAPHY/TANDEM MASS SPECTROMETRY (LC/MS/MS). EPA document #: EPA/600/R-18/352

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