RESTEK Pure Chromatography

Incorporating Ultrashort-Chain Compounds into the Comprehensive Analysis of PFAS in Potable and Non-Potable Waters

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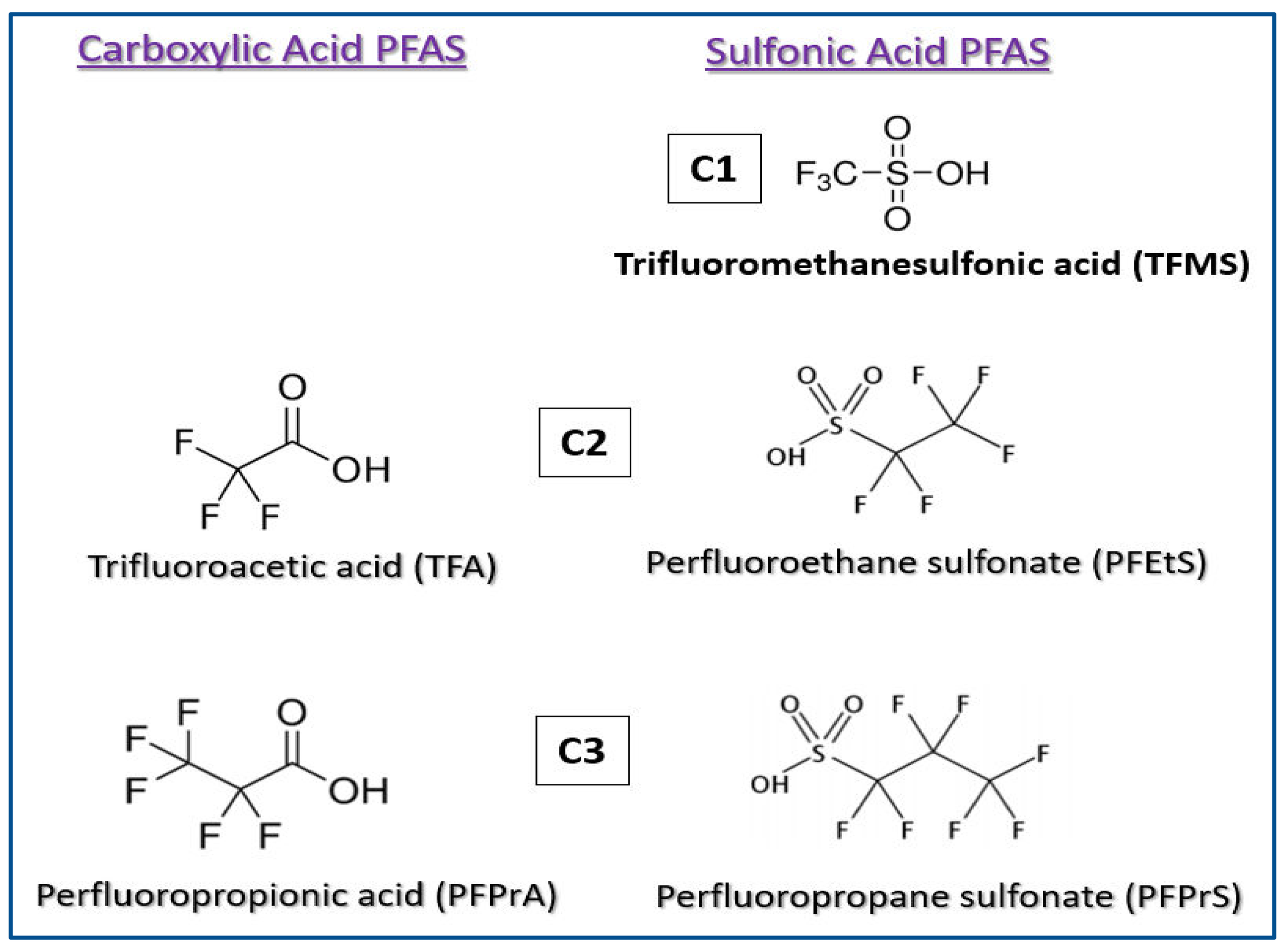
Introduction

Ultrashort-chain (USC) per- and polyfluoroalkyl substances (PFAS) are small and very polar compounds with carbon chain lengths shorter than C4. Their ubiquitous and high levels of occurrence in environmental aquatic systems are emerging as a significant concern, rivaling the well-established issues associated with long-chain PFAS contamination. Therefore, it is important to analyze both USC and long-chain PFAS together in water samples to comprehensively assess and address the full spectrum of PFAS contamination. The high polarity of USC PFAS poses a challenge for standard chromatographic practices in PFAS analysis, primarily due to insufficient chromatographic retention. In this study, a simple and reliable workflow was developed for the simultaneous analysis of C1 to C14 perfluoroalkyl carboxylic and sulfonic acids, along with other groups of PFAS, in both potable and non-potable waters. The chromatographic separation was conducted using a polar-embedded reversed-phase LC column with an inert coating on the hardware. A dilute-and-shoot workflow was evaluated by accuracy and precision analysis of fortified drinking waters and wastewaters. Additional potable and non-potable waters collected from various source waters were tested to further demonstrate that the established workflow is suitable for the accurate quantification of targeted PFAS in a wide range of water matrices.

Figure 1: Structures of C1 to C3 PFAS



Methods

Table 1: Analytical Conditions (Waters Xevo TQ-S with Acquity UPLC)

Analytical Column	Ultra Inert IBD 100 mm x 2.1 mm, 3 µm (Restek Cat.# 9175312-T)	
Delay Column	PFAS Delay Column (Restek Cat.# 27854)	
Mobile Phase A	5 mM ammonium formate, 0.1% formic acid in water	
Mobile Phase B	Acetonitrile	
Gradient	**Time (min)**	**%B**
	0.00	50
	7.00	95
	10.00	95
	10.01	50
	12.00	50
Flow Rate	0.4 mL/min	
Injection Volume	45 µL	
Column Temp.	40°C	
Ion Mode	Scheduled MRM with negative ESI	

Water Samples

Wastewater samples were gifts from GDIT (Falls Church, VA). These include a publicly owned treatment works (POTW), a hospital, a metal finisher, and a chemical manufacturer wastewater effluents. Bottled waters were obtained from local grocery stores. Tap waters were collected from the facility of Restek Corp. and local households served by different borough water authorities. In addition, a natural spring water, two well waters, and three creek waters were collected from central Pennsylvania regions. .

Conclusions

A simple and reliable dilute-and-shoot workflow was established in this study to provide a unique solution for incorporating ultrashort-chain compounds into a comprehensive measurement of PFAS in various water matrices. The reported method was sensitive, accurate, and precise by implementing an inert-coated polar-embedded alkyl phase column for chromatographic analysis. Most importantly, this solution can offer a valuable tool for monitoring these emergent PFAS in environmental water systems and assist in generating guidelines for future regulatory actions.

Standard and Sample Preparation

The calibration standard solutions (250 µL) were prepared in reverse osmosis water at the range of 1 to 1000 ng/L in the polypropylene HPLC vials. Five mass-labeled PFAS were implemented as quantitative internal standards (QIS) (see **Table 2**). A 2 µL aliquot of QIS working solution containing 40 ng/mL of $^{13}C_3$-PFBA, 20 ng/mL of $^{13}C_2$-PFHxA and $^{13}C_4$-PFOA, and 10 ng/mL of $^{13}C_5$-PFNA and $^{13}C_2$-PFDA, was added to each standard solution, followed by mixing with 250 µL of methanol containing 1% acetic acid.

Tap water, spring bottled water, and treated sewage wastewater effluent from a POTW (publicly owned treatment works) facility were used for the assessment of method accuracy and precision. Tap water and bottled water were used directly without filtration. POTW water (~ 10 mL) was filtered with polypropylene syringe filters and collected in 50-mL polypropylene tubes. These water samples (250 µL) were fortified at concentrations of 2, 4, 10, 50, and 250 ppt with native analytes and isotopically labeled ^{13}C-TFA, which served as a surrogate for the determination of TFA recovery. Each fortified sample was mixed with 2 µL of QIS working solution and 2.5 µL of extracted internal standards (EIS) working solution containing 10 ng/mL of mass-labeled PFAS (see **Table 2** for the list). A 250 µL aliquot of methanol containing 1% acetic acid was then added and mixed with fortified samples for LC-MS/MS analysis.

Results & Discussion

(1) **LC-MS/MS Method Development:** A chromatographic method was established (see **Table 1**) for the analysis of 45 PFAS compounds (**Figure 2**). The Ultra Inert IBD column exhibited satisfactory chromatographic performance under reverse-phased conditions. The inert-coated column showed a notable enhancement in detection sensitivity for most of the analytes. This improvement was evident by 3% to 75% increase in peak area and peak height. The MS/MS transition parameters for each analyte are provided in **Table 2**.

(2) **Linearity:** Employing quadratic regression (1/x weighted), all analytes exhibited acceptable linearities with r^2 >0.995 and deviations <30%. Table 2 shows differential linearity ranges of analytes, ranging from 1 ppt to 1000 ppt, with variation at the lowest calibration concentration.

(3) **Accuracy & Precision:** Three batches of analyses were conducted on different days, totaling nine repetitions at each fortified level. The average recovery and relative standard deviation (RSD) are presented in **Table 3**. All analytes exhibited recovery values within the range of 70 – 130% across all fortification levels. Satisfactory method precision was demonstrated with %RSD values within 20%. Additionally, the results indicated that all EIS had recovery values within 30% of the nominal concentration.

(4) **Measurement of 45 Targeted PFAS in Potable and Non-Potable Waters:** Each sample was prepared in triplicate with the addition of EIS. Consistent with the accuracy and precision analysis, the recoveries of EIS were within 30% of the nominal concentration (100 ppt) across all source waters. This demonstrated that the established method was suitable for accurate measurement of targeted PFAS in a wide range of water matrices (see results in **Table 4**).

Figure 2: Chromatogram for the Analysis of a 500 ppt Standard Solution

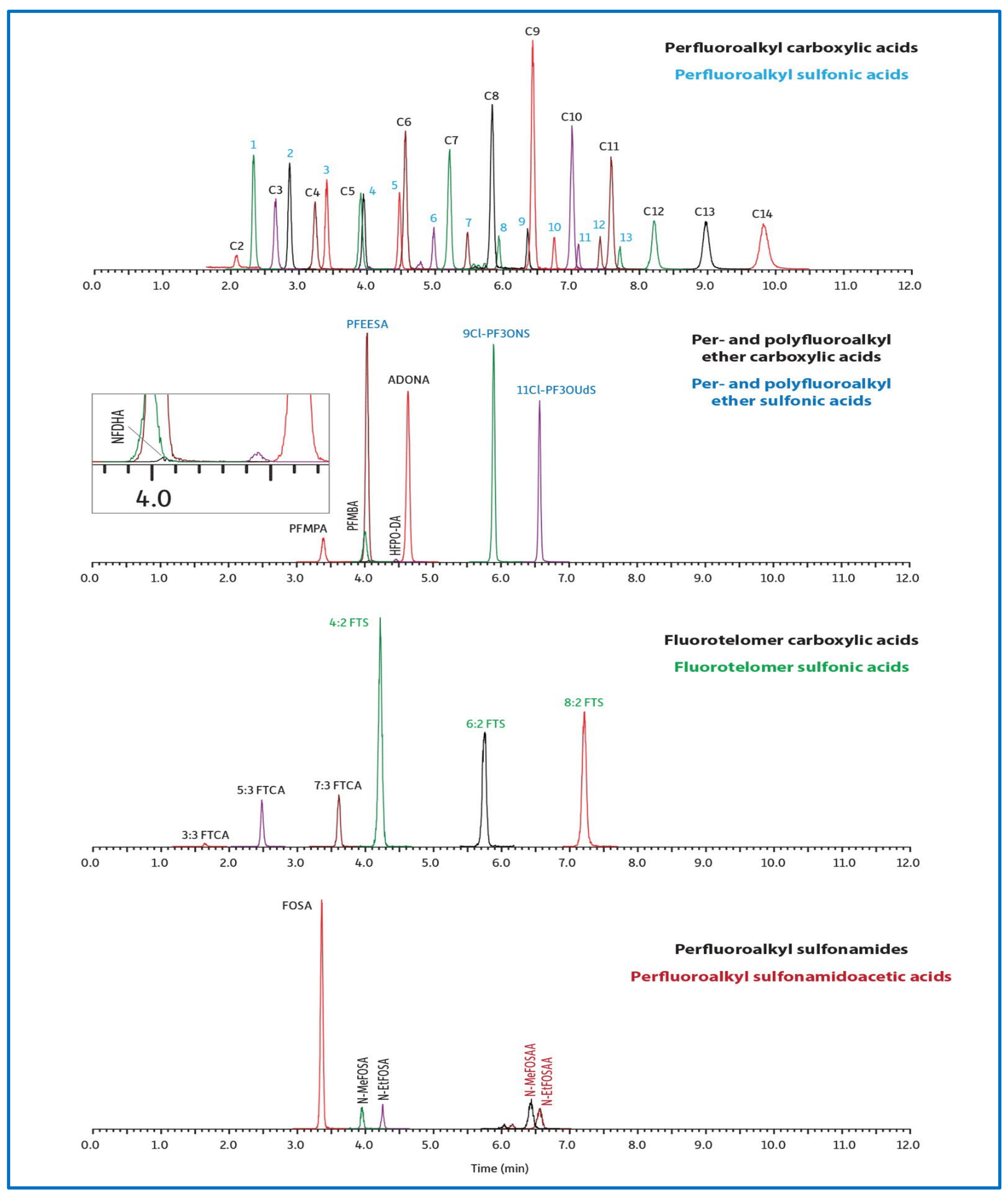


Table 2: MS Transitions and Analytes Retention Times

Compounds	Retention Time (min)	Precusor Ion	Product ions*	Cone (V)	Collision (V)	Quantification Internal Standard
Target Analytes						
Perfluoroalkyl carboxylic acids						
Trifluoroacetic acid (TFA)	2.12	113.03 [M-H]-	69.01	10	10	$^{13}C_3$-PFBA
Perfluoropropanoic acid (PFPrA)	2.69	162.97 [M-H]-	119.02	10	8	$^{13}C_3$-PFBA
Perfluorobutanoic acid (PFBA)	3.27	213.03 [M-H]-	168.98	14	8	$^{13}C_3$-PFBA
Perfluoropentanoic acid (PFPeA)	3.94	262.97 [M-H]-	218.97	2	6	$^{13}C_2$-PFHxA
Perfluorohexanoic acid (PFHxA)	4.59	313.10 [M-H]-	268.97/118.99	2	8/20	$^{13}C_2$-PFHxA
Perfluoroheptanoic acid (PFHpA)	5.24	363.16 [M-H]-	319.09/169.06	8	10/18	$^{13}C_4$-PFOA
Perfluorooctanoic acid (PFOA)	5.86	413.10 [M-H]-	368.96/168.90	2	10/16	$^{13}C_4$-PFOA
Perfluorononanoic acid (PFNA)	6.45	463.10 [M-H]-	419.01/219.02	4	10/16	$^{13}C_5$-PFNA
Perfluorodecanoic acid (PFDA)	7.03	513.17 [M-H]-	469.16/219.06	4	12/16	$^{13}C_2$-PFDA
Perfluoroundecanoic acid (PFUnA)	7.60	563.23 [M-H]-	519.24/269.07	6	12/18	$^{13}C_2$-PFDA
Perfluorododecanoic acid (PFDoA)	8.23	613.23 [M-H]-	569.19/169.06	8	12/26	$^{13}C_2$-PFDA
Perfluorotridecanoic acid (PFTrDA)	8.99	663.23 [M-H]-	619.21/169.06	8	14/28	$^{13}C_2$-PFDA
Perfluorotetradecanoic acid (PFTeDA)	9.83	712.67 [M-H]-	668.69/168.94	10	12/26	$^{13}C_2$-PFDA
Perfluoroalkyl sulfonic acids						
Trifluoromethanesulfonic acid (TFMS)	2.36	148.97 [M-H]-	79.93/98.92	62	18/18	$^{13}C_3$-PFBA
Perfluoroethanesulfonic acid (PFEtS)	2.89	198.90 [M-H]-	79.92/98.91	38	22/22	$^{13}C_3$-PFBA
Perfluoropropanesulfonic acid (PFPrS)	3.44	248.97 [M-H]-	79.92/98.91	2	24/24	$^{13}C_3$-PFBA
Perfluorobutanesulfonic acid (PFBS)	3.97	298.97 [M-H]-	79.97/98.89	2	26/26	$^{13}C_2$-PFHxA
Perfluoropentanesulfonic acid (PFPeS)	4.50	349.10 [M-H]-	79.98/98.98	6	32/30	$^{13}C_2$-PFHxA
Perfluorohexanesulfonic acid (PFHxS)	5.01	398.90 [M-H]-	79.97/98.89	56	32/34	$^{13}C_2$-PFHxA
Perfluoroheptanesulfonic acid (PFHpS)	5.50	449.17 [M-H]-	79.98/98.97	4	42/38	$^{13}C_4$-PFOA
Perfluorooctanesulfonic acid (PFOS)	5.96	499.03 [M-H]-	79.92/98.90	8	40/40	$^{13}C_4$-PFOA
Perfluorononanesulfonic acid (PFNS)	6.38	549.10 [M-H]-	79.92/98.83	12	42/40	$^{13}C_5$-PFNA
Perfluorodecanesulfonic acid (PFDS)	6.77	599.17 [M-H]-	79.98/98.83	8	44/46	$^{13}C_2$-PFDA
Perfluoroundecanesulfonic acid (PFUdS)	7.12	648.73 [M-H]-	79.94/98.94	38	50/44	$^{13}C_2$-PFDA
Perfluorododecanesulfonic acid (PFDoS)	7.44	698.77 [M-H]-	79.95/98.94	10	60/44	$^{13}C_2$-PFDA
Perfluorotridecanesulfonic acid (PFTrDS)	7.73	748.73 [M-H]-	79.94/98.94	8	76/52	$^{13}C_2$-PFDA
Fluorotelomer sulfonic acids						
1H,1H,2H,2H-Perfluorohexane sulfonic acid (4:2 FTS)	4.22	327.10 [M-H]-	307.08/80.83	50	18/24	$^{13}C_2$-PFHxA
1H,1H,2H,2H-Perfluorooctane sulfonic acid (6:2 FTS)	5.75	427.17 [M-H]-	407.18/80.71	2	22/32	$^{13}C_4$-PFOA
1H,1H,2H,2H-Perfluorodecane sulfonic acid (8:2 FTS)	7.22	527.17 [M-H]-	507.16/80.83	66	26/32	$^{13}C_2$-PFDA
Fluorotelomer carboxylic acids						
3-perfluoropropyl propanoic acid (3:3 FTCA)	1.64	241.00 [M-H]-	177.00/117.00	2	6/6	$^{13}C_3$-PFBA
3-perfluoropentyl propanoic acid (5:3 FTCA)	2.49	340.93 [M-H]-	216.96/236.93	2	24/14	$^{13}C_3$-PFBA
3-perfluoroheptyl propanoic acid (7:3 FTCA)	3.61	440.90 [M-H]-	336.88/316.91	20	12/22	$^{13}C_3$-PFBA
Perfluorooctane sulfonamides						
Perfluorooctanesulfonamide (FOSA)	3.36	498.17 [M-H]-	77.97/477.76	8	28/26	$^{13}C_3$-PFBA
N-methyl perfluorooctanesulfonamide (NMeFOSA)	3.96	511.77 [M-H]-	168.95/218.91	2	26/24	$^{13}C_2$-PFHxA
N-ethyl perfluorooctanesulfonamide (NEtFOSA)	4.26	525.83 [M-H]-	168.96/218.92	10	26/24	$^{13}C_2$-PFHxA
Perfluorooctane sulfonamidoacetic acids						
N-methyl perfluorooctanesulfonamidoacetic acid (NMeFOSAA)	6.44	570.20 [M-H]-	419.17/483.16	46	20/14	$^{13}C_5$-PFNA
N-ethyl perfluorooctanesulfonamidoacetic acid (NEtFOSAA)	6.56	584.20 [M-H]-	419.18/483.11	6	20/16	$^{13}C_5$-PFNA
Per- and Polyfluoroether carboxylic acids						
Perfluoro-3-methoxypropanoic acid (PFMPA)	3.40	228.93 [M-H]-	84.97/198.94	10	10/14	$^{13}C_3$-PFBA
Perfluoro-4-methoxybutanoic acid (PFMBA)	4.00	278.87 [M-H]-	84.96/234.93	8	10/6	$^{13}C_2$-PFHxA
Nonafluoro-3,6-dioxaheptanoic acid (NFDHA)	4.06	294.93 [M-H]-	200.91/85.02	8	4/22	$^{13}C_2$-PFHxA
Hexafluoropropylene oxide dimer acid (HFPO-DA)	4.46	285.03 [M-COOH]-	169.02/185.02	2	6/16	$^{13}C_2$-PFHxA
4,8-Dioxa-3H-perfluorononanoic acid (ADONA)	4.63	376.90 [M-H]-	250.93/84.97	22	12/26	$^{13}C_2$-PFHxA
Ether sulfonic acids						
Perfluoro(2-ethoxyethane)sulfonic acid (PFEESA)	4.04	314.83 [M-H]-	134.94/83.01	4	22/16	$^{13}C_2$-PFHxA
9-Chlorohexadecafluoro-3-oxanonane-1-sulfonic aicd (9Cl-PF3ONS)	5.88	530.78 [M-H]-	350.85/82.96	12	26/24	$^{13}C_4$-PFOA
11-Chloroeicosafluoro-3-oxaundecane-1-sulfonic acid (11Cl-PF3OUdS)	6.56	630.78 [M-H]-	450.80/82.95	8	26/32	$^{13}C_5$-PFNA
Extracted Internal Standards						
$^{13}C_3$-PFPrA	2.69	165.97 [M-H]-	120.96	10	11	$^{13}C_3$-PFBA
$^{13}C_4$-PFBA	3.27	217.03 [M-H]-	171.98	2	8	$^{13}C_3$-PFBA
$^{13}C_5$-PFPeA	3.94	267.97 [M-H]-	222.99	2	6	$^{13}C_2$-PFHxA
$^{13}C_5$-PFHxA	4.59	318.03 [M-H]-	272.93	2	7	$^{13}C_2$-PFHxA
$^{13}C_4$-PFHpA	5.24	366.90 [M-H]-	321.93	2	10	$^{13}C_4$-PFOA
$^{13}C_8$-PFOA	5.86	420.97 [M-H]-	375.94	2	10	$^{13}C_4$-PFOA
$^{13}C_6$-PFDA	7.03	518.90 [M-H]-	473.87	4	13	$^{13}C_2$-PFDA
$^{13}C_7$-PFUnA	7.60	569.90 [M-H]-	524.87	2	12	$^{13}C_2$-PFDA
$^{13}C_2$-PFDoA	8.23	614.84 [M-H]-	569.87	2	12	$^{13}C_2$-PFDA
$^{13}C_2$-PFTeDA	9.83	714.78 [M-H]-	669.80	8	14	$^{13}C_2$-PFDA
$^{13}C_3$-PFBS	3.97	301.97 [M-H]-	79.97	2	28	$^{13}C_2$-PFHxA
$^{13}C_3$-PFHxS	5.01	401.90 [M-H]-	79.97	2	36	$^{13}C_2$-PFHxA
$^{13}C_8$-PFOS	5.96	506.84 [M-H]-	79.97	4	42	$^{13}C_4$-PFOA
$^{13}C_2$-4:2 FTS	4.22	328.97 [M-H]-	308.96	2	18	$^{13}C_2$-PFHxA
$^{13}C_2$-8:2 FTS	7.22	528.90 [M-H]-	508.90	2	24	$^{13}C_2$-PFDA
$^{13}C_8$-FOSA	3.36	505.91 [M-H]-	77.95	4	32	$^{13}C_3$-PFBA
d3-NMeFOSAA	6.44	572.90 [M-H]-	418.91	50	18	$^{13}C_5$-PFNA
d5-NEtFOSAA	6.56	588.97 [M-H]-	418.86	48	20	$^{13}C_5$-PFNA
Quantification Internal Standards						
$^{13}C_3$-PFBA	3.27	215.97 [M-H]-	171.97	10	8	
$^{13}C_2$-PFHxA	4.59	314.97 [M-H]-	269.93	8	8	
$^{13}C_4$-PFOA	5.86	416.87 [M-H]-	371.88	2	8	
$^{13}C_5$-PFNA	6.45	467.87 [M-H]-	422.89	16	10	
$^{13}C_2$-PFDA	7.03	514.87 [M-H]-	469.84	8	10	

* Quantifier Ion/Qualifier Ion

Table 3: Accuracy & Precision Analysis of Fortified Water Samples

Analytes	Average Recovery (RSD, %), n=9					Average Recovery (RSD, %), n=9					Average Recovery (RSD, %), n=9				
	Tap Water					Bottled Water					POTW				
	Fortified Concentration (ng/L)					Fortified Concentration (ng/L)					Fortified Concentration (ng/L)				
	2	4	10	50	250	2	4	10	50	250	2	4	10	50	250
^{13}C-TFA	-	-	110 (9.61)	89.8 (5.10)	91.5 (2.04)	-	-	104 (15.6)	99.4 (8.09)	103 (7.45)	-	-	-	104 (9.46)	108 (8.57)
PFPrA	102 (6.88)	100 (3.72)	98.6 (6.71)	105 (8.98)	101 (6.85)	96.7 (5.90)	101 (6.64)	97.9 (6.08)	107 (3.13)	114 (7.77)	99.7 (3.96)	101 (11.9)	99.7 (9.18)	109 (3.90)	113 (1.99)
PFBA	108 (8.17)	107 (7.28)	104 (9.06)	104 (5.13)	103 (7.20)	96.4 (5.81)	94.7 (8.49)	90.2 (6.21)	103 (6.58)	112 (6.78)	100 (8.79)	98.0 (6.35)	99.2 (7.44)	104 (8.77)	106 (4.82)
PFPeA	109 (9.02)	115 (2.98)	105 (7.90)	111 (6.13)	107 (8.17)	93.2 (8.17)	99.1 (13.9)	95.5 (10.2)	105 (5.95)	111 (8.53)	104 (9.17)	110 (6.19)	101 (5.66)	109 (2.80)	116 (2.05)
PFHxA	88.2 (8.36)	99.8 (8.44)	92.0 (6.26)	105 (7.96)	103 (8.06)	100 (13.1)	96.5 (9.30)	91.0 (8.66)	99.5 (4.92)	108 (8.20)	91.8 (12.1)	98.5 (10.0)	92.9 (9.53)	101(3.30)	103 (6.53)
PFHpA	88.7 (6.44)	101 (8.38)	86.2 (6.26)	95.1 (6.97)	91.2 (7.28)	96.9 (8.26)	92.3 (3.67)	87.3 (4.82)	97.9 (6.15)	104 (5.56)	115 (5.90)	111 (8.16)	97.6 (6.90)	97.1 (5.74)	99.5 (4.58)
PFOA	111 (6.58)	117 (4.67)	103 (9.51)	104 (8.34)	101 (8.98)	94.4 (10.9)	100 (10.8)	101 (8.29)	105 (6.09)	112 (6.11)	108 (8.67)	105 (8.15)	101 (4.86)	105 (4.68)	109 (5.20)
PFNA	108 (7.53)	110 (5.46)	97.8 (3.83)	104 (6.23)	99.5 (8.40)	108 (9.34)	103 (8.32)	97.3 (3.99)	105 (5.46)	112 (7.09)	113 (8.50)	117 (5.50)	95.1 (5.73)	103 (6.97)	107 (4.67)
PFDA	99.4 (6.34)	104 (5.56)	95.1 (5.35)	98.6 (9.37)	95.8 (8.66)	101 (11.9)	96.9 (6.73)	92.2 (8.25)	100 (5.31)	109 (8.86)	108 (10.6)	111 (8.44)	91.8 (5.90)	97.6 (4.10)	101 (3.49)
PFUnA	110 (14.0)	109 (11.4)	108 (14.6)	107 (8.05)	95.5 (7.14)	109 (10.6)	104 (8.74)	90.6 (11.0)	97.7 (9.52)	105 (5.72)	106 (12.6)	102 (9.97)	95.1 (8.99)	97.7 (3.90)	101 (6.28)
PFDoA	103 (14.2)	104 (9.98)	96.5 (14.1)	101 (5.81)	102 (3.95)	97.5 (5.77)	95.2 (4.93)	78.5 (1.90)	85.1 (5.14)	103 (5.68)	98.4 (16.6)	107 (9.05)	93.0 (3.83)	111 (11.9)	112 (12.2)
PFTrDA	101 (13.3)	91.1 (11.0)	87.5 (7.09)	82.3 (5.23)	86.5 (3.05)	106 (9.03)	100 (8.97)	81.8 (13.1)	87.8 (18.6)	98.2 (9.05)	94.1 (15.9)	94.4 (13.2)	79.7 (9.70)	90.3 (11.3)	96.7 (13.5)
PFTeDA	103 (6.04)	91.2 (10.6)	90.1 (8.18)	86.5 (10.9)	93.4 (4.21)	116 (3.97)	109 (6.74)	90.5 (8.94)	93.5 (18.2)	114 (5.74)	113 (12.7)	97.5 (18.9)	82.9 (12.4)	95.2 (13.3)	104 (18.0)
TFMS	112 (9.16)	108 (10.4)	97.3 (8.16)	105 (6.42)	104 (7.25)	101 (9.04)	107 (6.85)	96.7 (4.30)	106 (2.88)	112 (7.17)	104 (15.6)	108 (7.24)	94.9 (5.45)	94.9 (5.32)	96.0 (1.88)
PFEtS	103 (8.31)	115 (5.52)	103 (3.25)	106 (4.64)	107 (5.60)	102 (7.45)	105 (4.66)	97.8 (3.00)	106 (2.01)	111 (7.50)	93.1 (15.3)	108 (7.71)	87.9 (6.50)	95.7 (4.51)	97.9 (2.89)
PFPrS	109 (9.22)	114 (7.23)	99.3 (8.52)	106 (7.76)	107 (7.32)	101 (10.4)	106 (7.28)	98.1 (6.13)	108 (1.98)	111 (6.44)	105 (9.36)	114 (4.26)	91.5 (4.65)	99.5 (3.97)	102 (4.11)
PFBS	109 (6.89)	109 (10.7)	94.3 (8.59)	101 (5.45)	102 (6.53)	103 (13.7)	101 (9.53)	85.8 (5.98)	101 (2.59)	108 (8.90)	93.4 (12.3)	107 (6.18)	91.8 (7.88)	100 (5.38)	105 (6.90)
PFPeS	104 (5.33)	113 (3.79)	97.9 (4.84)	106 (7.29)	104 (9.30)	95.6 (10.3)	102 (5.75)	92.3 (5.80)	102 (2.79)	109 (9.05)	102 (13.3)	113 (8.62)	90.2 (4.13)	99.7 (2.68)	103 (4.89)
PFHxS	84.1 (16.7)	105 (7.50)	90.8 (12.8)	104 (4.37)	102 (3.77)	110 (8.75)	99.4 (8.55)	90.9 (11.8)	96.5 (2.79)	103 (8.67)	89.3 (17.7)	95.2 (8.96)	100 (12.7)	98.6 (6.64)	105 (6.83)
PFHpS	111 (7.72)	108 (6.82)	99.7 (7.04)	108 (5.65)	105 (6.59)	99.8 (8.79)	94.2 (8.80)	90.9 (7.75)	105 (5.47)	110 (8.06)	85.1 (16.1)	109 (9.59)	96.0 (7.89)	106 (3.56)	111 (2.42)
PFOS	112 (7.55)	106 (7.10)	95.5 (10.2)	107 (7.39)	107 (6.83)	111 (12.9)	93.5 (8.65)	91.8 (9.70)	106 (6.02)	109 (6.08)	79.0 (18.5)	107 (6.22)	86.1 (8.60)	101 (7.45)	110 (4.62)
PFNS	117 (13.8)	104 (10.7)	91.9 (10.2)	104 (4.92)	99.1 (6.15)	102 (12.8)	90.8 (15.2)	86.8 (10.4)	101 (8.80)	112 (6.74)	104 (9.28)	92.5 (14.2)	85.0 (9.21)	98.9 (4.69)	108 (3.95)
PFDS	107 (15.0)	106 (8.32)	94.4 (17.2)	97.9 (11.1)	94.4 (3.40)	96.9 (19.1)	105 (12.1)	89.3 (11.4)	103 (10.2)	107 (5.82)	109 (11.1)	106 (11.0)	92.6 (13.1)	101 (7.80)	101 (4.53)
PFUdS	108 (13.5)	92.4 (15.5)	88.1 (1.58)	85.7 (2.32)	93.4 (3.38)	101 (18.5)	100 (16.3)	87.3 (10.5)	92.9 (14.5)	105 (5.71)	95.6 (18.8)	102 (8.93)	77.9 (7.72)	90.2 (8.96)	96.4 (7.42)
PFDoS	114 (13.4)	96.5 (11.9)	85.9 (5.01)	83.5 (11.6)	93.9 (2.71)	114 (7.52)	106 (10.7)	84.8 (14.6)	90.7 (14.5)	108 (7.49)	111 (9.06)	95.0 (10.7)	80.0 (13.7)	83.1 (8.45)	99.5 (12.4)
PFTrDS	91.0 (17.8)	72.5 (18.2)	72.0 (13.8)	72.9 (14.4)	84.6 (3.55)	126 (1.13)	109 (14.4)	86.2 (17.1)	88.4 (19.0)	112 (5.51)	94.1 (14.9)	107 (15.1)	79.8 (12.5)	85.2 (12.4)	96.4 (15.1)
4:2 FTS	106 (8.72)	109 (8.83)	90.2 (13.0)	103 (9.27)	101 (10.2)	103 (11.0)	98.1 (16.3)	88.6 (10.1)	94.3 (4.60)	108 (10.3)	122 (5.65)	113 (4.55)	91.5 (7.23)	100 (3.92)	104 (5.01)
6:2 FTS	108 (8.94)	112 (6.81)	96.4 (17.3)	102 (4.45)	99.4 (7.60)	108 (6.44)	95.2 (13.7)	88.0 (13.3)	97.7 (9.07)	106 (7.53)	110 (10.3)	109 (12.0)	93.1 (10.0)	95.2 (7.65)	102 (5.42)
8:2 FTS	111 (13.4)	107 (12.1)	92.6 (11.3)	101 (5.28)	94.6 (5.86)	112 (10.5)	109 (5.14)	95.0 (3.66)	103 (3.89)	109 (8.72)	116 (10.0)	102 (16.1)	89.3 (12.6)	101 (5.81)	106 (3.58)
3:3 FTCA	-	-	-	83.7 (8.92)	82.6 (5.64)	-	-	-	95.4 (10.4)	105 (6.94)	-	-	-	-	-
5:3 FTCA	-	120 (6.07)	106 (12.0)	103 (8.99)	103 (8.78)	-	103 (8.78)	94.3 (12.1)	105 (6.32)	109 (8.62)	-	115 (7.21)	104 (8.42)	108 (7.38)	108 (5.05)
7:3 FTCA	-	107 (8.36)	91.4 (16.2)	105 (7.98)	106 (7.36)	-	115 (5.16)	98.9 (9.92)	102 (8.75)	110 (7.09)	-	122 (6.51)	92.6 (18.9)	99.7 (9.76)	105 (5.88)
FOSA	107 (9.41)	107 (5.20)	95.4 (8.59)	95.7 (4.63)	95.5 (6.05)	111 (7.75)	103 (8.73)	91.6 (3.72)	104 (3.88)	112 (7.06)	110 (8.60)	101 (10.9)	79.1 (4.69)	89.4 (5.01)	96.6 (6.21)
NMeFOSA	-	-	106 (12.9)	105 (6.50)	104 (9.06)	-	-	105 (8.01)	101 (10.8)	115 (5.88)	-	-	110 (18.8)	92.1 (10.3)	116 (3.63)
NEtFOSA	-	-	105 (14.7)	112 (4.89)	105 (7.49)	-	-	121 (9.43)	100 (13.0)	110 (8.06)	-	-	116 (9.55)	103 (11.9)	104 (11.6)
NMeFOSAA	-	123 (7.06)	88.5 (14.6)	102 (8.37)	99.5 (7.89)	-	109 (12.1)	106 (10.1)	92.9 (13.8)	104 (9.53)	-	118 (10.3)	98.2 (12.1)	98.8 (9.01)	100 (6.96)
NEtFOSAA	-	-	106 (10.9)	96.1 (11.1)	92.6 (5.99)	-	-	101 (15.7)	100 (10.3)	105 (8.11)	-	-	106 (10.9)	96.1 (11.1)	92.6 (5.99)
PFMPA	99.0 (15.9)	103 (10.6)	90.2 (6.11)	103 (8.22)	103 (8.21)	99.5 (9.11)	99.6 (11.0)	92.2 (4.76)	103 (4.57)	112 (7.29)	94.3 (11.0)	105 (7.54)	88.4 (7.38)	98.1 (3.33)	102 (4.66)
PFMBA	105 (7.67)	107 (8.82)	95.8 (7.63)	107 (6.27)	103 (7.01)	92.3 (9.01)	102 (9.17)	90.1 (8.50)	100 (4.51)	109 (7.70)	85.9 (7.17)	99.9 (10.5)	87.0 (8.69)	101 (4.18)	109 (5.75)
NFDHA	-	-	-	115 (9.78)	115 (8.61)	-	-	-	111 (6.59)	111 (7.73)	-	-	-	90.5 (13.9)	114 (3.75)
HFPO-DA	-	-	115 (13.1)	108 (5.70)	106 (7.76)	-	-	106 (12.3)	101 (10.1)	112 (6.19)	-	-	111 (6.49)	92.5 (16.2)	95.6 (12.4)
ADONA	94.4 (11.5)	109 (5.71)	98.4 (7.58)	106 (7.56)	104 (8.94)	97.3 (11.4)	101 (6.41)	91.6 (3.35)	100 (4.26)	107 (10.3)	90.8 (12.6)	116 (5.19)	90.9 (4.78)	103 (3.45)	106 (5.37)
PFEESA	102 (8.88)	113 (4.75)	98.8 (7.11)	108 (6.06)	105 (8.76)	101 (8.99)	105 (8.33)	93.6 (5.67)	102 (3.03)	110 (9.16)	89.4 (12.7)	113 (8.74)	92.8 (1.95)	102 (1.80)	108 (3.07)
9Cl-PF3ONS	100 (8.99)	107 (4.54)	95.7 (2.88)	105 (6.31)	104 (9.09)	100 (8.53)	101 (7.16)	90.2 (4.28)	105 (4.22)	112 (8.47)	95.4 (10.3)	102 (9.40)	85.4 (6.64)	101 (4.97)	106 (4.67)
11Cl-PF3OUdS	88.2 (12.3)	96.8 (7.36)	87.8 (8.81)	96.7 (4.65)	95.1 (4.17)	91.0 (11.1)	96.8 (6.21)	85.0 (4.94)	100 (11.8)	108 (5.75)	95.1 (8.68)	105 (3.84)	82.7 (4.07)	97.5 (7.82)	101 (6.36)

Table 4: Measurement of 45 Targeted PFAS in Various Water Matrices

Water Samples	Averaged Concentration (ng/L)												
	Ultrashort-Chain			Short-Chain						Long-Chain		Alternatives	
	TFA	PFPrA	TFMS	PFBA	PFBS	PFPeA	PFHxA	PFHxS	PFHpA	PFOA	PFOS	PFMPA	HFPO-DA
Potable Waters													
Tap Water #1	176	2.66	8.40	nd*	nd	< 1.00	2.13	nd	nd	< 1.00	nd	nd	nd
Tap Water #2	317	1.54	7.14	nd	2.25	nd	nd	nd	nd	nd	< 2.00	nd	nd
Tap Water #3	166	3.15	10.9	nd	2.14	2.51	1.24	nd	nd	< 1.00	4.76	nd	nd
Tap Water #4	330	5.48	12.8	nd	1.68	1.97	nd	nd	nd	nd	nd	nd	nd
Tap Water #5	1186	29.0	25.4	13.2	8.58	13.7	17.7	nd	5.78	18.0	5.63	nd	nd
Bottled Water #1 (spring water)	107	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
Bottled Water #2 (spring water)	257	1.66	< 1.00	< 2.00	1.21	nd	nd	nd	nd	nd	< 2.00	nd	nd
Bottled Water #3 (RO purified)	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
Natural Spring Water	486	2.91	4.81	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
Well Water #1	557	1.82	1.74	nd	nd	nd	nd	nd	nd	< 1.00	nd	nd	nd
Well Water #2	171	1.16	< 1.00	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
Non-Potable Waters													
Creek Water #1	605	4.88	6.75	5.82	19.5	3.50	1.52	nd	< 1.00	< 1.00	6.06	4.40	nd
Creek Water #2	626	3.07	2.26	nd	2.68	nd	nd	nd	nd	nd	< 2.00	nd	nd
Creek Water #3	627	10.9	8.28	< 2.00	2.19	4.94	2.35	nd	nd	3.08	5.97	nd	nd
POTW Water Effluent	1156	24.2	9.66	nd	2.84	6.50	24.0	2.28	< 1.00	12.9	3.88	nd	nd
Hospital Effluent	487	3.08	1.45	nd	nd	2.15	1.50	nd	nd	nd	nd	nd	nd
Metal Finisher Effluent	678	2.78	8.89	2.87	3.11	2.52	2.09	nd	nd	< 1.00	112	nd	nd
Chemical Manufacture Effluent	90,473	8,540	13.3	62.8	1.13	100	7.22	nd	12.0	20.8	nd	14.0	5,709

*non-detected

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