

Determination of PFAS in Drinking Water by LC-MS/MS according to GB 5750.8-2023

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Abstract

This method for the simultaneous determination of 27 PFAS (per-and polyfluoroalkyl substances) in drinking water by ultra-high performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS) was established in accordance with GB 5750.8-2023. Water samples were enriched and concentrated using a weak anion exchange (WAX) solid phase extraction column. For all 27 analytes, an excellent linear response was observed in the range of 5 to 200 μ g/L (injected standard solutions), and the correlation coefficient R² was greater than 0.9950 for each molecule. The limits of quantitation for 27 PFAS compounds in the water samples were 2.97-4.92 ng/L. The recoveries were 79.0-83.4% and the relative standard deviations were 1.6-4.6%.

Introduction

PFAS are persistent organic compounds that exist widely in the environment. Recent awareness has drawn attention to the toxicity of these substances. Liquid chromatography-mass spectrometry (LC-MS) is a common technique for the determination of perfluoroalkyl substances.¹⁻⁵

In the new version of the Chinese national standard for drinking water, GB 5750.8-2023⁶, sections 84 and 85 designate 11 PFAS compounds as critical target analytes for drinking water testing.

Part 84 of GB 5750.8 stipulates 11 perfluorinated compounds to be analyzed, which are PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFBS, PFHxS, PFHpS, and PFOS. The sample pretreatment method, LC-MS/MS method conditions, and qualitative and quantitative ion information are described in detail.

Part 85 of GB 5750.8 requires only the determination of PFOS (**Figure 1**). The sample pretreatment method and other method details are the same as for section 84.

The required Limit of Quantification (LOQ) for the analytes is given with 5 ng/L, and the linear concentration range for the external calibration is given with 5.0-200 μ g/L (representing concentrations in the water sample of 5-200 ng/L considering the sample pre-treatment enrichment factor of 1:1000) with linearity R² >0.9950.

In this study, 27 PFAS target compounds (**Table 1**), including PFBA, PFMPA, PFPeA, and PFMOBA, were selected for detection and analysis in drinking water based on the guidelines in the updated standard GB 5750.8-2023 and target compounds established by the EPA. Method verification indicators and internal quality control were implemented in accordance with the provisions of the GB 5750.8-2023 method.

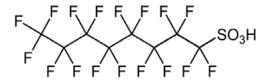


Figure 1. Example PFAS (chemical structure of perfluorooctanesulfonic acid, PFOS)



Table 1. PFAS analytes in scope of this study (* marked are in GB method)

Compound no.	Compound name	Compound abbreviation	CAS No.
1*	Heptafluorobutyric acid	PFBA	375-22-4
2	Perfluoro-3-methoxypropanoic acid	PFMPA	377-73-1
3*	Perfluorovaleric acid	PFPeA	2706-90-3
4*	Perfluorobutanesulfonic acid	PFBS	375-73-5
5	2,2,3,3,4,4-Hexafluoro-4-(trifluoromethoxy)butanoic acid	PFMOBA	863090-89-5
6	Perfluoro(2-ethoxyethane)sulfonic acid	PFEESA	113507-82-7
7	Perfluoro-3,6-dioxaheptanoic acid	3,6-OPFHpA	151772-58-6
8	1H,1H,2H,2H-Perfluorohexanesulfonic acid	4:2 FTSA	757124-72-4
9*	Perfluorohexanoic acid	PFHxA	307-24-4
10	Perfluoropentanesulfonic acid hydrate	PFPeS	2706-91-4
11	Perfluoro-2-(propyloxy)propionic acid	HFPO-DA	13252-13-6
12*	Perfluoroheptanoic acid	PFHpA	375-85-9
13*	Perfluorohexanesulfonic acid	PFHxS	3871-99-6
14	4,8-dioxa-3H-Perfluorononanoic acid	ADONA	919005-14-4
15	1H,1H,2H,2H-Perfluorooctanesulfonic acid	6:2 FTSA	27619-97-2
16*	Perfluoroheptanesulfonic acid	PFHpS	375-92-8
17*	Perfluorooctanoic acid	PFOA	335-67-1
18*	Perfluorooctanesulfonic acid	PFOS	2795-39-3
19*	Perfluorononanoic acid	PFNA	375-95-1
20*	Perfluorodecanoic acid	PFDA	335-76-2
21	Sodium 1H,1H,2H,2H-perfluorodecane sulfonate	8:2 FTSA	27619-96-1
22	N-Methylperfluorooctanesulfonamidoacetic acid	N-MeFOSAA	2355-31-9
23	Perfluoroundecanoic acid	PFUnDA	2058-94-8
24	N-Ethylperfluorooctane sulfonamidoacetic acid	EtFOSAA	2991-50-6
25	Perfluorododecanoic acid	PFDoDA	307-55-1
26	Pentacosafluorotridecanoic acid	PFTrDA	72629-94-8
27	Perfluorotetradecanoic acid	PFTeDA	376-06-7

Experimental

Standard, Sample and Reagent Preparation

Reagent solutions, standards, and samples were prepared according to the following procedures as described in the GB method.

Reagent Preparation

Aqueous methanol (30/70): Combine 30 mL methanol and 70 mL water and mix well (prepare freshly).

Ammonia solution in aqueous methanol (0.1%): Add 500 μ L ammonia (28.0-30.0% NH3) to a 500 mL volumetric flask, fill to the mark with aqueous methanol and mix well (prepare fresh).

Ammonium acetate aqueous solution (0.025 mol/L): Dissolve 0.9635 g ammonium acetate in 500 mL water, mix well, and adjust to pH 4 with acetic acid (\geq 99.8%).

Ammonium acetate aqueous solution ($0.005 \, \text{mol/L}$): Dissolve 0.3854 g ammonium acetate in 1 L water and mix well. Use this solution as mobile phase A.

Standard Preparation

PFAS stock solution I (1000 mg/L): Dissolve 10.0 mg of each of the 27 PFAS reference materials in 10 mL methanol. Keep the resulting solution at 0 $^{\circ}$ C to 4 $^{\circ}$ C; it can be stored for three months.

PFAS stock solution II (10 mg/L): Pipette 1 mL of PFAS stock solution II into a 100 mL amber glass volumetric flask and fill up to mark with methanol. Store at 0 °C to 4 °C and protected from light.

PFAS stock solution III (1 mg/L): Pipette 1 mL of PFAS stock solution II into a 10 mL amber glass volumetric flask and fill up to mark with methanol. Store at 0 °C to 4 °C and protected from light.

PFAS standard solutions 1-5: Prepare a total of five standard working solutions (nos. 1-5) by pipetting 5 μL , 10 μL , 50 μL , 100 μL , and 200 μL , respectively, of PFAS stock solution III into five separate 1 mL vials. Fill vials up to mark with methanol. The concentration of PFAS in the resulting solutions are 5.0, 10.0, 50.0, 100, and 200 $\mu g/L$, respectively.

Sample Preparation

Water sample: Dissolve 4.625 g ammonium acetate in 1 L of the water sample to be analyzed and mix well. The pH of the resulting water sample is 6.8-7.0.

Extraction by SPE

- Conditioning: Connect SPE-WAX solid phase extraction tube bed wt. 500 mg, volume 6 mL (Supelclean™ ENVI-WAX™, 54057-U) to a PTFE free Visiprep™ SPE vacuum manifold (57030-U), and condition with 5 mL ammonia-methanol solution (0.1%), 7 mL methanol and re-equilibrate with 10 mL water.
- Loading: Pipette pre-treated sample (1 L) onto SPE the tube; in order not to negatively affect recovery rates, a flow rate of 8 mL/min must not be exceeded.
- Washing: After the sample is finished (Step 2 complete), wash sample with 5 mL ammonium acetate aqueous solution (0.025 mol/L) followed by 12 mL water.
- Drying: Dry SPE-WAX solid phase extraction tube for 15 min under vacuum.
- 5. Elution: Elute with 5 mL methanol and 7 mL ammonia solution in methanol. Collect eluate in a 15 mL polypropylene centrifuge tube.
- 6. Evaporation & reconstitution: Blow down samples to almost complete dryness using nitrogen and a water bath (temperature ≤ 40 °C). Reconstitute with aqueous methanol (30/70) to result in 1 mL sample volume and vortex. This represents and enrichment of 1:1000.

Spiking experiments

For the determination of method recovery (%) and precision, prepare two samples by mixing 1 L of drinking water sample with 30 μ L and 50 μ L of PFAS stock solution III, respectively. The concentration of PFAS in the two samples is 30 ng/L (utilized for the analysis of precision) and 50 ng/L (recovery).

LC-MS/MS Analysis

Contamination by PFAS compounds originating from the HPLC system and materials used in analysis is a concern. Therefore, a highly retentive Ascentis® Express PFAS Delay column was placed in front of the injector to provide retention of PFAS compounds originating from the mobile phase system across various mobile phase conditions. It delays the instrument background and prevents interference with peaks originating from the analyzed/injected samples.

For the separation, a Fused-Core® Ascentis® Express PFAS HPLC column was used, which is application tested for PFAS analysis to provide reliable and efficient separations.

The obtained sample extracts and standards were analyzed by LC-MS/MS using the parameters described in **Tables 2 & 3**.

Table 2. LC-MS/MS Conditions used for PFAS analysis in drinking water

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LC Conditions		
Instrument:	Waters [™] Acquity I-class plus and Waters [™] Xevo [™] TQS UPS -tandem mass spectrometer equipped with electrospray ionization (ESI) source.	
Column:	Ascentis® Express 90 Å PFAS, 2.7 μ m , 10 cm \times 2.1 mm I.D. (53559-U)	
Delay column:	Ascentis® Express 90 Å PFAS Delay, 2.7 μm, 5 cm × 3.0 mm I.D. (53572-U)	
Mobile phase:	[A] 5 mM Ammonium acetate in water; [B] Methanol	
Gradient:	Time (min)	% В
	0.0	33.0
	18.0	98.0
	18.1	100.0
	21.0	100.0
	21.1	33.0
	26.0	33.0
Flow rate:	0.30 mL/min	
Column temp.:	35 °C	<u> </u>
Detection:	MS/MS, ESI(-), MRM (Table 3)	
Injection:	5.0 μL	

Table 3. MS Conditions used for PFAS detection

MS Parameter	
Polarity:	ESI (-)
Capillary voltage :	4.0 kV
Atomization gas flow::	3.0 mL/min
Heater flow	10.0 mL/min
Heat block temperature:	400 °C
DL tube temperature :	250 °C
Interface temperature :	300 °C
Scan:	Multiple reaction monitoring (MRM) See Table 4

Results & Discussion

Drinking water samples were pre-treated with ammonium acetate, prepared by solid phase extraction (SPE), and analyzed by UHPLC-MS/MS, with the MS being operated in MRM mode. The 27 PFAS target analytes were quantified using an external standard calibration.

Figures 2 and 3 show MRM chromatograms (MS operated in negative ESI mode) of the analysis of PFAS stock solution III and a drinking water sample spiked with PFAS stock solution III at a concentration of 50 ng/L of each PFAS. In Figure 4, the result for an unspiked drinking water sample is displayed.

Table 4 lists the MRM transition used and the chromatographic data obtained by the analysis of a spiked drinking water sample shown in Figure 3.

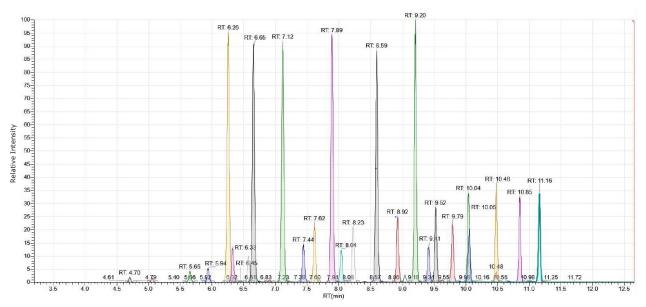


Figure 2. LC-MS/MS chromatogram of PFAS standard solution (c= $50 \mu g/L$).

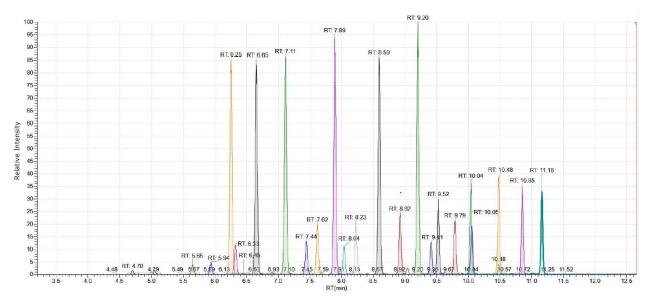


Figure 3. LC-MS/MS chromatogram of a drinking water sample spiked with PFAS stock solution III at a concentration of 50 ng/L of each PFAS.

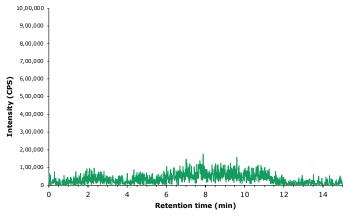


Figure 4. LC-MS/MS chromatogram of an unspiked drinking water sample.

Table 4. Chromatographic data and MRM transitions for the analysis of a drinking water sample spiked with PFAS at a concentration of 50 ng/L of each PFAS

Compound	Retention time (min)	MRM Transitions m/z
PFBA	4.70	213→169
PFMPA	4.79	327→307
PFPeA	5.65	263→219
PFMOBA	5.93	449→80
PFBS	6.25	299→80
4:2FTSA	6.32	230→85
3,6-OPFHpA	6.45	295→80
PFHxA	6.57	313→269
PFEESA	6.65	349→80
HFPO-DA	6.89	285→169
PFPeS	7.11	315→135
PFHpA	7.44	363→319
ADONA	7.62	377→251
PFHxS	7.89	399→80
6:2FTSA	8.03	498→78
PFOA	8.22	413→369
PFHpS	8.58	279→85
PFNA	8.91	463→419
PFOS	9.19	499→80
8:2FTSA	9.40	549→80
PFDA	9.52	513→469
N-MeFOSAA	9.78	570→419
PFUnDA	10.03	563→519
EtFOSAA	10.04	584→419
PFDoDA	10.47	613→569
PFTrDA	10.85	663→619
PFTeDA	11.15	713→669

Calibration

The external calibration for all 27 PFAS using 5 PFAS standard solutions (c = 5.0, 10.0, 50.0, 100, and $200~\mu g/L$) provided R² linearity values between 0.9982 and 0.9999.

As an example, the results of the calibration for PFBA are displayed in **Figure 5** and **Table 5**. All other PFAS provided similar results (see the table in the appendix).

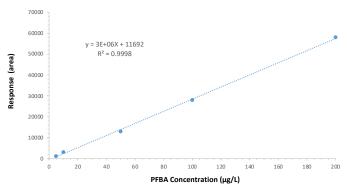


Figure 5. Calibration curve obtained by the analysis of PFBA standard solutions 1-5 (c = 5.0, 10.0, 50.0, 100, and 200 μ g/L).

Table 5. Calibration data for PFBA as an example obtained by the analysis of PFAS standard solutions 1-5 (c = 5.0, 10.0, 50.0, 100, and 200 μ g/L)

Sample	PFBA concentration (µg/L)	Area
PFAS standard solution 1	5.0	1161
PFAS standard solution 2	10.0	2998
PFAS standard solution 3	50.0	12990
PFAS standard solution 4	100.0	27980
PFAS standard solution 5	200.0	57960

Data Precision and Recovery (%)

The drinking water sample with a PFAS concentration of 30 ng/L was used for evaluation of method precision (n=7), while the second sample (PFAS concentration 50 ng/L) was used to assess method recovery (n=6). Summarized results obtained are shown in **Table 6**. For precision, the % RSD ranged from 1.6 to 4.6%, and the recovery rates were between 79.0 and 83.4%.

Table 6. Average precision %RSD (n=7) for a 30 ng/L spiked sample and the average recovery (n=6) for a 50 ng/L spiked sample

Compound	Precision 30 ng/L Sample pound (n=7)		Average Recovery 50 ng/L Sample (n=6)	
	Average (µg/L)	RSD (%)	%	
PFBA	27.3	1.6	81.3	
PFMPA	27.0	2.1	80.9	
PFPeA	26.7	2.4	82.5	
PFBS	26.8	2.4	82.6	
PFMOBA	26.2	2.9	82.1	
PFEESA	27.5	3.1	79.9	
3,6-OPFHpA	27.1	2.9	80.4	
4:2 FTSA	26.0	3.7	83.4	
PFHxA	27.9	1.9	82.8	
PFPeS	26.6	2.5	80.9	
HFPO-DA	28.1	3.5	81.1	
PFHpA	26.3	3.8	83.1	
PFHxS(µg/L)	26.7	3.7	81.7	
ADONA	27.3	1.6	82.4	
6:2 FTSA	28.1	2.6	81.3	
PFHpS	25.3	2.2	80.6	
PFOA	27.9	3.8	82.0	
PFOS	27.5	2.6	79.0	
PFNA	26.4	1.2	82.8	
PFDA	27.0	2.9	81.5	
8:2 FTSA	27.8	3.7	80.5	
N-MeFOSAA	27.8	2.8	82.7	
PFUnDA	28.2	3.4	81.0	
EtFOSAA	26.5	4.6	80.5	
PFDoDA	26.9	2.0	82.8	
PFTrDA	27.7	3.8	81.3	
PFTeDA	26.7	4.1	80.5	

Sensitivity

For the sensitivity determination for the LC method, the baseline noise of a blank drinking water sample was employed: 3N/X was used to determine Limit of Detection (LOD), and 10N/X was used to determine Limit of Quantification (LOQ). LODs ranged from 0.99-1.64 µg/L and LOQ from 2.97-4.92 µg/L for the LC method (**Table 7**) representing concentrations in the water samples of 0.99-1.64 ng/L and 2.97-4.92 ng/L respectively.

Table 7. LOQ & LOD of 27 PFAS compounds in water samples

Compound no.	Compound	LOD (ng/L)	LOQ (ng/L)
1	PFBA	1.05	3.15
2	PFMPA	1.13	3.39
3	PFPeA	1.14	3.42
4	PFBS	1.08	3.24
5	PFMOBA	1.61	4.83
6	PFEESA	1.62	4.86
7	3,6-OPFHpA	1.15	3.45
8	4:2 FTSA	1.13	3.39
9	PFHxA	1.59	4.77
10	PFPeS	0.99	2.97
11	HFPO-DA	1.16	3.48
12	PFHpA	1.09	3.27
13	PFHxS	1.11	3.33
14	ADONA	1.52	4.56
15	6:2 FTSA	1.55	4.65
16	PFHpS	1.07	3.21
17	PFOA	1.61	4.83
18	PFOS	1.09	3.27
19	PFNA	1.04	3.12
20	PFDA	1.07	3.21
21	8:2 FTSA	1.09	3.27
22	N-MeFOSAA	1.11	3.33
23	PFUnDA	1.64	4.92
24	EtFOSAA	1.02	3.06
25	PFDoDA	1.12	3.36
26	PFTrDA	1.09	3.27
27	PFTeDA	1.10	3.30

Conclusion

A method for the simultaneous determination of 27 PFAS in drinking water by UHPLC-MS/MS using a Fused-Core® Ascentis® Express PFAS column was developed. An Ascentis® Express PFAS Delay column was installed to prevent instrument background interferences. Water samples were enriched and concentrated by SPE using a Supelclean™ ENVI-WAX™ weak anion exchange tube.

The 27 PFAS showed for the external calibration a good linear relationship in the range of 5-200 μ g/L (representing, considering the applied sample preparation, a water sample concentration of 5-200 ng/L), and the correlation coefficients R² were greater than 0.9950. The recoveries were 79.0-83.4%, the relative standard deviations were 1.6-4.6%, and the limits of quantitation (LOQ) for the LC method for 27 PFAS compounds were 2.97-4.92 μ g/L, representing concentrations in the water samples of 2.97-4.92 ng/L.

The method performed excellently regarding selectivity, peak shape, and necessary retention and can therefore be used for the detection and analysis of PFAS in drinking water in accordance with the GB 5750.8-2023 standard with high accuracy and reliability.

References

- Llorca M, et al. Development and validation of a pressurized liquid extraction liquid chromatography-tandem mass spectrometry method for perfluorinated compounds determination in fish. J. Chrom A, 2009;1216(43):7195-7204. https://doi.org/10.1016/j. chroma.2009.06.062
- Li Z, et al. Perfluoroheptanoic acid induces Leydig cell hyperplasia but inhibits spermatogenesis in rats after pubertal exposure. Toxicology 2020;448:152633-152633. https://doi.org/10.1016/j. tox.2020.152633
- Arvaniti SO, et al. Simultaneous determination of eighteen perfluorinated compounds in dissolved and particulate phases of wastewater, and in sewage sludge by liquid chromatographytandem mass spectrometry. Analytical Methods: Advancing Methods and Applications 2014;6(5):1341-1349. https://doi. org/10.1039/C3AY42015A
- Vavrous A, et al. Method for analysis of 68 organic contaminants in food contact paper using gas and liquid chromatography coupled with tandem mass spectrometry. Food Control 2016;60:221-229. https://doi.org/10.1016/j.foodcont.2015.07.043
- Pérez F, et al. Accumulation of perfluoroalkyl substances in human tissues. Environment International 2013;59:354-362. https://doi. org/10.1016/j.envint.2013.06.004
- GB 5750.8-2023 Standard test methods for drinking water -Part 8: Indicators of organic matter. http://down.foodmate.net/ standard/sort/3/137087.html

Featured Products

Description	Cat. No.
HPLC Column	
Ascentis® Express 90 Å PFAS, 2.7 μm, 10 cm x 2.1 mm	53559-U
Ascentis® Express 90 Å PFAS Delay column, 2.7 µm, 5 cm × 3.0 mm I.D.	53572-U
Sample Preparation, Solvents and Reagents	
Supelclean™ ENVI-WAX™ SPE Tube, suitable for PFAS testing, bed wt. 500 mg, volume 6 mL, pk of 30 ea	54057-U
Visiprep [™] SPE, standard, 12-port model, PTFE free	57030-U
Millex® polyethersulfone (PES) syringe filter pore size 0.22 µm, diam. 13 mm, non-sterile, hydrophilic	SLGPX13NL
Methanol for UHPLC-MS LiChrosolv®	1.03726
Water for UHPLC-MS LiChrosolv®	1.03728
Ultrapure water from Milli-Q® IQ 7 series water purification system	ZIQ7005T0C
Ammonia (28.0-30.0% $\mathrm{NH_3}$), ACS reagent, 28.0-30.0% $\mathrm{NH_3}$ basis	221228
Acetic acid, puriss. p.a., ACS reagent, reag. ISO, reag. Ph. Eur., ≥99.8%	33209/ 33209-M
Ammonium acetate LiChropur $^{\mbox{\scriptsize TM}},$ eluent additive for LC-MS	73594
Certified Reference Materials TraceCERT® (* unless specified)	otherwise
Perfluorobutanoic acid (PFBA), neat, 10mg	75930
Perfluoro-3-methoxypropanoic acid (PFMPA), neat, 25 mg	73014
Perfluorovaleric acid (PFPeA), neat, 10 mg	73551
Perfluorobutanesulfonic acid (PFBS), neat, 25 mg	93634
Perfluoro-3,6-dioxaheptanoic acid (3,6-OPFHpA), neat, 50 mg	04292
Perfluorohexanoic acid (PFHxA), neat, 25 mg	93899
Perfluoro-2-(propyloxy)propionic acid (HFPO-DA), neat, 25 mg	94275
Perfluoroheptanoic acid (PFHpA), neat, 25 mg	93983
1H,1H,2H,2H-Perfluorooctanesulfonic acid (6:2 FTSA), neat, 25 mg	93497
Perfluoroheptanesulfonic acid (PFHpS), neat, 10 mg	78049
Perfluorooctanoic acid (PFOA), neat, 25 mg	93973
Perfluorooctanesulfonic acid (PFOS), 100 $\mu g/mL$ in methanol, analytical standard*	33607
Perfluorononanoic acid (PFNA), neat, 10 mg	05167
Perfluorodecanoic acid (PFDA), neat, 10 mg	91367
Perfluoroundecanoic acid (PFUnDA), neat, 10 mg	89988
N-Ethylperfluorooctane sulfonamidoacetic acid (EtFOSAA), neat, 25 mg	94707
Perfluorododecanoic acid (PFDoDA), neat, 10 mg	76467
Pentacosafluorotridecanoic acid (PFTrDA), neat, 10 mg	76705
Perfluorotetradecanoic acid (PFTeDA), neat, 10 mg	38400

Related Products

Description	Cat. No.
Acetonitrile tested for EPA533 and EPA537.1 PFAS Methods LiChrosolv®	1.04726
Methanol tested for EPA533 and EPA537.1 PFAS Methods LiChrosolv®	1.04732
Water tested for EPA533 and EPA537.1 PFAS Methods LiChrosolv®	1.04735

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Appendix

Complete calibration data for all 27 PFAS obtained by the analysis of PFAS standard solutions 1-5 (c = 5.0, 10.0, 50.0, 100 and 200 $\mu g/L$)

Compound no.	Compound	Calibration	Linearity
1	PFBA	y = 3E + 06x + 11692	$R^2 = 0.9998$
2	PFMPA	y = 1.80E+02X-1.50E+04	$R^2 = 0.9998$
3	PFPeA	y = 4.16E+02X+1.91E+05	$R^2 = 0.9982$
4	PFBS	y = 9.54E+03X+1.09E+06	$R^2 = 0.9983$
5	PFMOBA	y = 5.39E+02X+5.02E+04	$R^2 = 0.9993$
6	PFEESA	y = 9.65E + 03X + 5.80E + 05	$R^2 = 0.9993$
7	3,6-OPHpA	y = 7.53E+01X-1.41E+04	$R^2 = 0.9995$
8	4:2 FTSA	y = 1.38E + 03X + 7.02E + 04	$R^2 = 0.9987$
9	PFHxA	y = 1.01E + 03X + 1.15E + 05	$R^2 = 0.9991$
10	PFPeS	y = 9.84E + 03X + 7.04E + 05	$R^2 = 0.9989$
11	HFPO-DA	y = 1.05E+02X-5.62E+03	$R^2 = 0.9997$
12	PFHpA	y = 1.58E+03X+6.15E+04	$R^2 = 0.9993$
13	PFHxS	y = 1.04E + 04X + 4.98E + 05	$R^2 = 0.9988$
14	ADONA	y = 2.31E + 03X + 4.67E + 04	$R^2 = 0.9995$
15	6:2 FTSA	y = 1.32E + 03X + 1.94E + 05	$R^2 = 0.9994$
16	PFHpS	y = 9.47E + 03X + 5.95E + 04	$R^2 = 0.9993$
17	PFOA	y = 2.26E + 03X + 2.04E + 05	$R^2 = 0.9992$
18	PFOS	y = 1.00E + 04X + 2.18E + 04	$R^2 = 0.9992$
19	PFNA	y = 2.70E + 03X + 3.07E + 04	$R^2 = 0.9995$
20	PFDA	y = 3.04E + 03X - 1.77E + 04	$R^2 = 0.9988$
21	8:2 FTSA	y = 1.53E+03X-2.58E+04	$R^2 = 0.9999$
22	N-MeFOSAA	y = 2.72E+03X-3.15E+05	$R^2 = 0.9996$
23	PFUnDA	y = 3.51E+03X-3.22E+04	$R^2 = 0.9989$
24	EtFOSAA	y = 2.28E + 03X - 1.00E + 05	$R^2 = 0.9996$
25	PFDoA	y = 4.00E + 03X - 4.28E + 05	$R^2 = 0.9993$
26	PFTrDA	y = 3.53E + 03X - 8.02E + 05	$R^2 = 0.9985$
27	PFTeDA	y = 3.49E + 03X - 1.16E + 06	$R^2 = 0.9995$

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