Application Note

Environmental

Agilent

Trusted Answers

Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous Samples Per EPA Method 1633

Using the Agilent 6470 triple quadrupole mass spectrometer

Authors

Kathy Hunt and Ralph Hindle
Vogon Laboratory Services Ltd.
Cochrane, AB, Canada

Tarun Anumol,
Matthew Giardina, and
Emily Parry
Agilent Technologies, Inc.

Abstract

The United States (US) Environmental Protection Agency (EPA) Method 1633 is an analysis method for the detection and quantitation of per- and polyfluoroalkyl substances (PFAS) in a variety of matrices including wastewater, soils, solids, and tissues. This application note addresses PFAS testing in aqueous wastewater samples per the EPA method using optimized solid-phase sample extraction and LC/MS/MS analysis with the Agilent 1290 Infinity II liquid chromatograph (LC) system coupled to the Agilent 6470 triple quadrupole (TQ) mass spectrometer. This study verified method development and performance in terms of analyte extraction recoveries, linearity, sensitivity (method detection limits), and reproducibility.

Introduction

Many methods are used to perform the analyses of PFAS in drinking water, nondrinking water, soil, sediments, landfill leachate, and other potentially complex matrices. EPA Method 1633 is an isotope dilution method that strives to standardize the methodology for the quantitation of forty PFAS across nine compound classes – including linear and branched isomers – in nonpotable aqueous, solid, biosolid, and tissue samples. In addition to some emerging classes of PFAS, all analytes listed in EPA drinking water Methods 533 and 537.1 are included in the method. While samples are prepared and extracted according to their matrices, all the methods specify solid-phase extraction (SPE) using weak anion exchange and carbon cleanup.

This application note addresses PFAS in aqueous matrices and highlights the results of initial performance tests including linearity, precision, recovery, and detection limits, which were run on a 1290 Infinity II LC system coupled to a 6470 triple quadrupole LC/MS. Method performance for the analysis of wastewater effluent was also evaluated. The method was followed closely; only permitted changes in supplies, SPE cartridges, and instrumentation parameters were made. As noted in the method, the sample size analyzed was 500 mL.

Experimental

Consumables and supplies

To assist laboratories in preparing to run the method, a list of all Agilent consumables used in the production of this application note is provided in Appendix Table 6.

Extraction procedure

The extraction procedure for aqueous samples described in EPA Method 1633 was followed (Figure 1) for reagent water and wastewater effluent grab samples. Unpreserved 500 mL aqueous samples were fortified with surrogates (extracted internal standards (EIS)). Agilent weak anion exchange (WAX) solid-phase extraction cartridges (150 mg) packed with silanized glass wool were conditioned with methanolic ammonium hydroxide followed by formic acid. Samples were loaded onto the SPE cartridges at a slow flow rate and rinsed with reagent water and 1:1 formic acid:methanol.[2] The sample bottles were rinsed, and cartridges eluted with 1% methanolic ammonium hydroxide. The eluate was treated with acetic acid and cleaned up with loose carbon. After centrifugation, the samples were filtered through a nylon syringe filter into a collection tube containing internal standard (nonextracted internal standard (NIS)).

LC/TQ instrument conditions

LC/MS/MS analysis was performed using a 1290 Infinity II LC system coupled to a 6470 LC/TQ. The LC configuration and method parameters are shown in Table 1. A PFAS-specific delay column was placed between the pump and multisampler to separate background contaminants from compounds originating in the sample vial without significantly increasing backpressure. The system was controlled by Agilent MassHunter Acquisition Software. The mobile phases were matched to the EPA Method 1633 for consistency, though the gradient was simplified to increase throughput, while maintaining the separation needed in the method. The MS method parameters (Table 2) were optimized using the Agilent Source Optimizer. Dynamic multiple reaction monitoring (dMRM) in negative electrospray ionization mode was used for data acquisition. dMRM methods for Agilent triple quadrupole instruments enable accurate quantification of exceedingly narrow peaks from fast 1290 Infinity UHPLC separations for multi-analyte assays. The number of MRM transitions is adjusted dynamically throughout the LC run, selecting only transitions with relevant retention time windows. The analyte transitions selected (provided in Appendix Table 7) were similar to those listed in the method. Data were processed using MassHunter Quantitative Analysis Software.

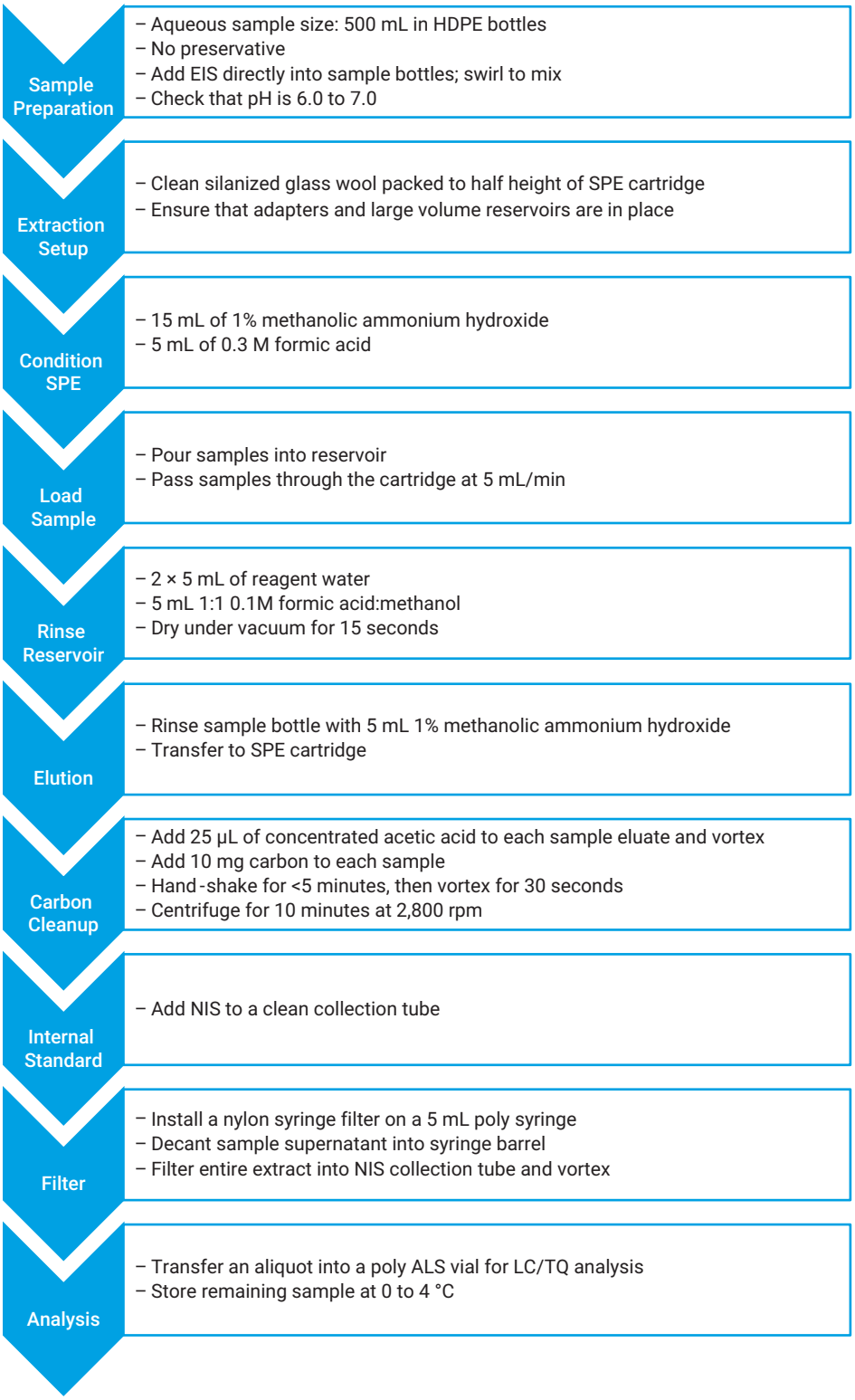

Figure 1. Extraction procedure.

Table 1. LC instrument conditions.

Parameter	Value
LC	Agilent 1290 Infinity II LC System with High Speed Pump (p/n G7120A), Multisampler (p/n G7167B), and Multicolumn Thermostat (MCT) thermostatted column compartment (p/n G7116B)
Guard Column	Agilent ZORBAX Eclipse Plus C18, 2.1 × 5 mm, 1.8 µm (p/n 821725-901)
Analytical Column	Agilent ZORBAX Eclipse Plus C18, 2.1 × 100 mm, 1.8 µm (p/n 959758-902)
Delay Column	Agilent InfinityLab PFC Delay Column, 4.6 × 30 mm (p/n 5062-8100)
Column Temperature	40 °C
Injection Volume	5 µL
Mobile Phase	A) 2 mM Ammonium acetate in 95% water (LC grade), 5% acetonitrile B) Acetonitrile (LC grade)
Gradient Flow Rate	0.4 mL/min
Gradient	Time (min) %B 0.0 2 0.2 2 10 95
Stop Time	12.2 min
Post Time	2.0 min

Table 2. TQ instrument conditions.

Parameter	Value
MS	Agilent 6470B TQ with Agilent Jet Stream ESI source
Source Parameters	
Gas Temperature	230 °C
Gas Flow	6 L/min
Nebulizer	20 psi
Sheath Gas Temperature	355 °C
Sheath Gas Flow	10 L/min
Capillary Voltage (Neg)	2,500 V
Nozzle Voltage (Neg)	0 V

Calibration standards

Analytical standard mixes were purchased from Wellington Laboratories. Subsequent combination and dilution of the standards were performed to prepare a high calibrator (Level 10) with analyte concentrations closely mirroring those in the high calibration standard of the method. A series of dilutions was prepared to a final calibrator concentration below that of the low standard in the method.

Results and discussion

Calibration performance

Instrument linearity was established per the method guidelines. All analytes had stable retention times with RSDs less than 3% across eight batches, and as shown in Table 3, excellent R^2 values of greater than 0.998, and relative standard errors (RSE) of less than 10% for an eight-point curve using quadratic fit with 1/x weighting and a forced origin. The MRM chromatogram shown in Figure 2 demonstrates good separation and detection of the target PFAS even at the low calibrator levels.

Bile salts separation

EPA Method 1633 specifies that "analytical conditions must be set to allow a separation of at least 1 minute between the bile salts (TDCA) and PFOS." The chromatographic and other analytical conditions used in this study met these criteria with TDCA and PFOS eluting at 5.7 and 7.1 minutes, respectively.

Surrogate recoveries

Extracted surrogate recovery in reagent water for n = 23 replicates (lab reagent blanks, precision and accuracy spikes, and low-level spikes for determining MDL) ranged from 66 to 122%, with RSDs of less than 15%. Twenty-two of the 24 surrogates had recoveries between 70 to 130%, which met typical EPA requirements. D_3-NMeFOSA and D_5 NEtFOSA showed slightly low recoveries of 66%, which agrees with the findings in the method.

Table 3. Calibration performance metrics for PFAS analyzed per EPA Method 1633.

Analyte	Average RT (n = 8)	Average R^2 (n = 8)	Average RSE for 8pt calibration curve (n = 8)	Low Calibrator Concentration (ng/mL)	High Calibrator (Level 8) (ng/mL)
PFBA	3.39	0.9988	6.5	0.5	62.5
PFPeA	4.48	0.9997	5.6	0.2	31.3
PFHxA	5.15	0.9996	4.7	0.1	15.6
PFHpA	5.67	0.9994	6.6	0.1	15.6
PFOA	6.13	0.9994	7.0	0.1	15.6
PFNA	6.55	0.9995	6.9	0.1	15.6
PFDA	6.96	0.9997	5.8	0.1	15.6
PFUnA	7.35	0.9996	5.9	0.1	15.6
PFDoA	7.74	0.9994	7.2	0.1	15.6
PFTrDA	8.11	0.9996	5.7	0.1	15.6
PFTeDA	8.48	0.9995	6.1	0.1	15.6
PFBS	5.22	0.9996	6.2	0.1	15.6
PFPeS	5.82	0.9992	6.8	0.1	15.6
PFHxS	6.32	0.9993	8.5	0.1	15.6
PFHpS	6.75	0.9994	6.8	0.1	15.6
PFOS	7.12	0.9995	6.2	0.1	15.6
PFNS	7.58	0.9994	7.9	0.1	15.6
PFDS	7.96	0.9994	7.3	0.1	15.6
PFDoS	8.69	0.9994	9.3	0.1	15.6
4:2 FTS	4.94	0.9993	6.4	0.5	62.5
6:2 FTS	5.93	0.9992	6.2	0.5	62.5
8:2 FTS	6.76	0.9990	7.9	0.5	62.5
PFOSA	8.59	0.9994	6.5	0.1	15.6
NMeFOSA	9.89	0.9993	8.9	0.1	15.6
NEtFOSA	10.23	0.9994	6.1	0.1	15.6
NMeFOSAA	7.01	0.9995	6.0	0.1	15.6
NEtFOSAA	7.16	0.9993	7.0	0.1	15.6
NMeFOSE	9.78	0.9995	7.0	1.2	156.3
NEtFOSE	10.12	0.9993	9.2	1.2	156.3
HFPO-DA	5.36	0.9994	7.7	0.5	62.5
ADONA	5.84	0.9997	5.0	0.5	62.5
PFMPA	3.90	0.9997	5.2	0.2	31.3
PFMBA	4.72	0.9996	6.0	0.2	31.3
NFDHA	5.09	0.9990	8.6	0.2	31.3
9Cl-PF3ONS	7.48	0.9997	5.3	0.5	62.5
11Cl-PF3OUdS	8.25	0.9997	5.5	0.5	62.5
PFEESA	5.51	0.9993	6.7	0.2	31.3
3:3 FTCA	4.20	0.9997	5.3	0.5	62.5
5:3 FTCA	5.61	0.9996	5.9	2.4	312.5
7:3 FTCA	6.66	0.9996	6.1	2.4	312.5

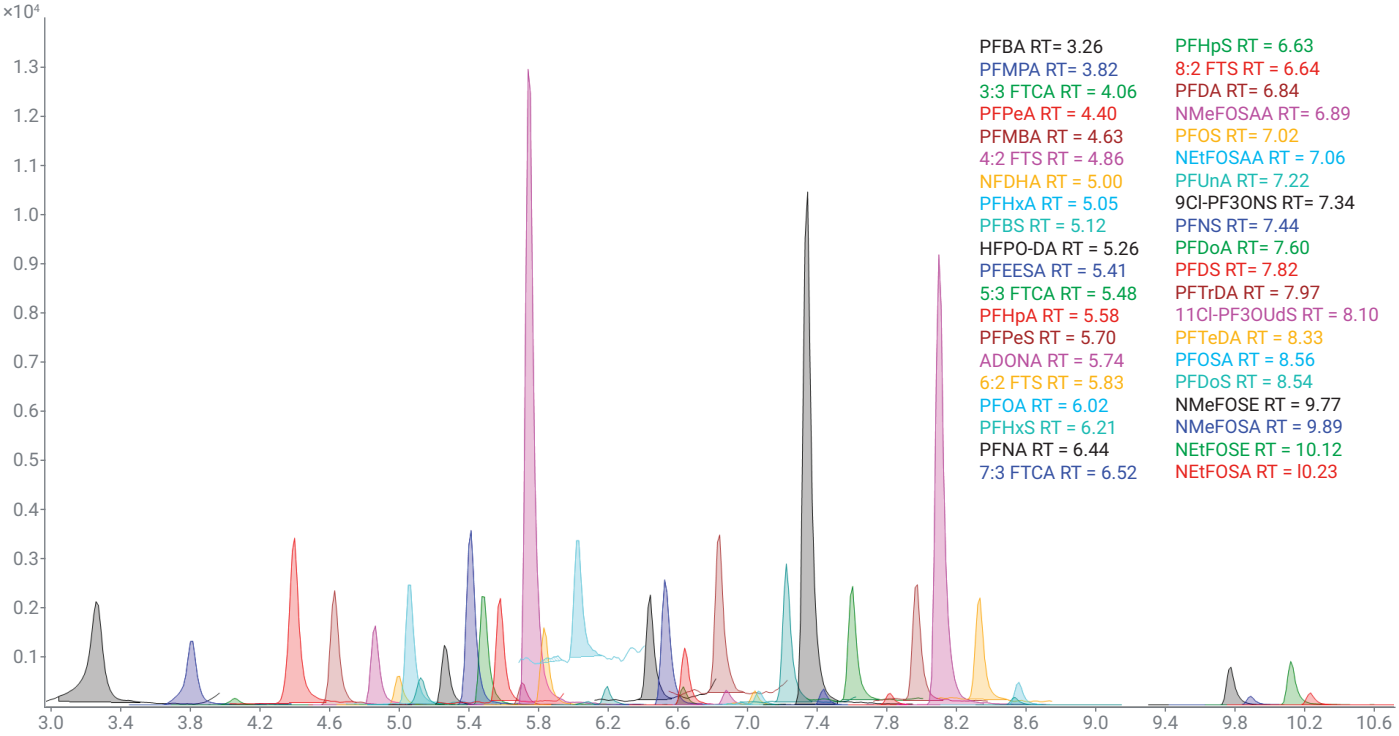

Figure 2. MRM chromatogram of PFAS in reagent water spiked at the low calibrator concentrations.

Method detection limits

Method detection limits (MDLs) were determined according to the MDL procedure in 40 CFR Part 136, Appendix B. The initial MDLs achieved on the 6470 LC/TQ following extraction of low-level spikes and lab reagent blanks (LRB) shown in Table 4 are equivalent or better than those documented by the multi-laboratory validation described in the method. MDLs for 32 of the PFAS were lower than 1 ng/L. The extracted blank levels were well below the levels listed in the method.

Precision and accuracy

Precision and accuracy extraction studies at the mid-level concentration produced excellent reproducibility. All RSDs were less than 9% and most recoveries (expressed as accuracy) fell between 75 and 125%.

Wastewater effluent samples

To demonstrate the real-world applicability of EPA Method 1633, four replicates of a wastewater effluent grab sample were spiked with all target analytes and extracted following the method procedure. The average background levels found in two replicates of unspiked wastewater (blanks) shown in Figure 3 were subtracted from the measured concentration in the spiked samples and the accuracy calculated. The results listed in Table 5 were consistent with the results obtained for the reagent water experiments. The RSDs were good and recoveries (expressed as accuracy) ranged from 64 to 159% (Table 5). Surrogate recoveries in seven replicates from two different wastewater effluent grab samples and spikes were generally between 50 to 150% (for $^{13}C_2$-4:2 FTS, average recovery was 152%). Good reproducibility (3 to 12%) was also obtained.

Table 4. Initial MDLs following extraction of low-level spikes and lab reagent blanks (LRB).

Analyte	Blank (ng/mL)	Initial MDL (ng/L)	EPA Method 1633 MDL (ng/L)
PFBA	<0.1	0.64	0.33
PFPeA	<0.1	0.23	0.20
PFHxA	<0.01	0.09	0.32
PFHpA	<0.01	0.20	0.22
PFOA	<0.01	0.11	0.30
PFNA	<0.01	0.18	0.22
PFDA	<0.01	0.17	0.33
PFUnA	<0.01	0.12	0.26
PFDoA	<0.1	0.13	0.38
PFTrDA	<0.1	0.21	0.24
PFTeDA	<0.1	0.22	0.26
PFBS	<0.01	0.15	0.25
PFPeS	<0.01	0.16	0.20
PFHxS	<0.1	0.23	0.22
PFHpS	<0.01	0.18	0.14
PFOS	<0.1	0.26	0.33
PFNS	<0.01	0.20	0.30
PFDS	<0.1	0.18	0.33
PFDoS	<0.1	0.26	0.18
4:2 FTS	<0.01	0.74	2.28

Analyte	Blank (ng/mL)	Initial MDL (ng/L)	EPA Method 1633 MDL (ng/L)
6:2 FTS	<0.01	0.55	3.97
8:2 FTS	<0.01	0.57	1.57
PFOSA	<0.1	0.21	0.23
NMeFOSA	<0.1	0.29	0.20
NEtFOSA	<0.01	0.12	0.59
NMeFOSAA	<0.1	0.44	0.59
NEtFOSAA	<0.1	0.41	0.32
NMeFOSE	<1	1.53	1.19
NEtFOSE	<1	1.88	1.02
HFPO-DA	<0.1	0.61	0.41
ADONA	<0.01	0.46	0.78
PFMPA	<0.01	0.26	0.14
PFMBA	<0.01	0.36	0.18
NFDHA	<0.01	0.45	0.12
9Cl-PF3ONS	<0.01	0.74	1.38
11Cl-PF3OUdS	<0.2	0.72	0.87
PFEESA	<0.01	0.34	0.82
3:3 FTCA	<0.01	1.08	0.72
5:3 FTCA	<0.1	1.90	5.07
7:3 FTCA	<0.2	3.12	5.94

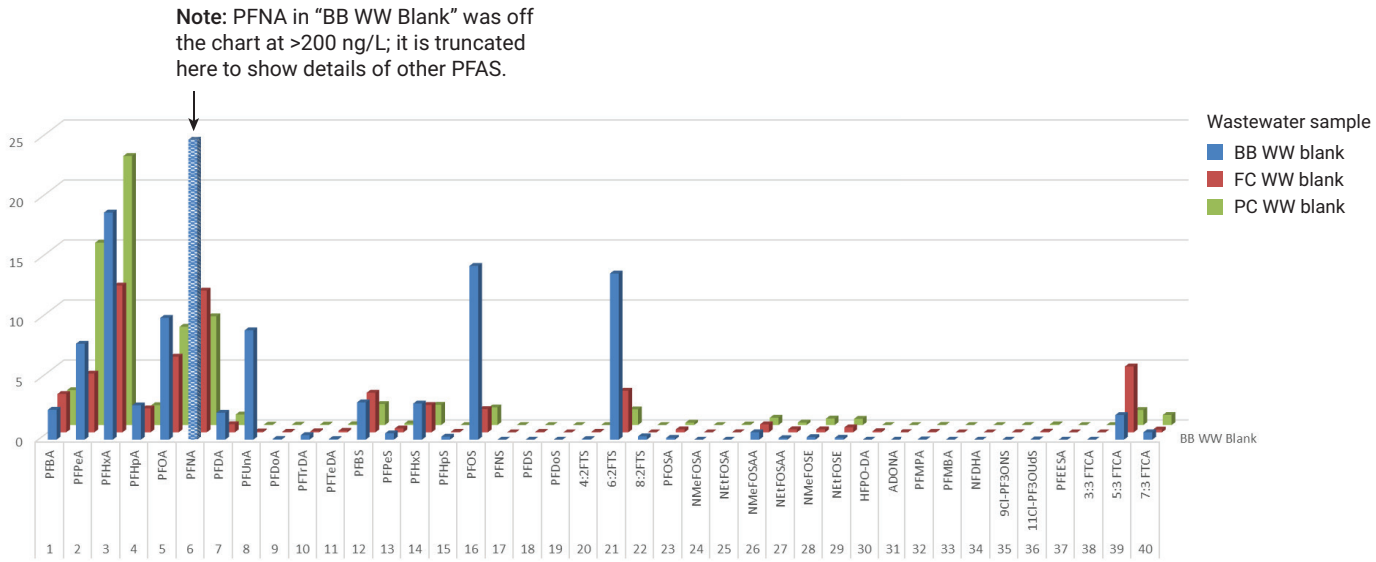

Figure 3. PFAS detected in three unique wastewater effluent samples.

Table 5. Background concentration of PFAS in wastewater effluent blanks and calculated recoveries (expressed as accuracy).

Analyte	Average Conc Detected in WW Blank (ng/L)	Spiked Concentration (ng/L)	Background Subtracted Extracted Concentration (ng/L)	Accuracy
PFBA	3.2	50.0	52.7	105%
PFPeA	15.2	25.0	25.4	102%
PFHxA	22.6	12.5	12.9	103%
PFHpA	1.6	12.5	12.6	101%
PFOA	8.4	12.5	12.5	100%
PFNA	8.8	12.5	12.7	102%
PFDA	0.9	12.5	12.6	101%
PFUnA	0.0	12.5	12.5	100%
PFDoA	0.0	12.5	12.4	100%
PFTrDA	0.0	12.5	12.5	100%
PFTeDA	0.1	12.5	12.5	100%
PFBS	1.9	12.5	12.9	103%
PFPeS	0.2	12.5	12.2	98%
PFHxS	1.5	12.5	12.8	103%
PFHpS	0.1	12.5	13.3	106%
PFOS	1.6	12.5	12.0	96%
PFNS	–	12.5	10.3	82%
PFDS	–	12.5	9.6	77%
PFDoS	0.0	12.5	8.0	64%
4:2 FTS	0.0	50.0	52.3	105%
6:2 FTS	1.3	50.0	50.8	102%
8:2 FTS	0.1	50.0	50.7	101%
PFOSA	0.2	12.5	13.0	104%
NMeFOSA	–	12.5	13.4	107%
NEtFOSA	0.1	12.5	12.5	100%
NMeFOSAA	0.6	12.5	13.2	105%
NEtFOSAA	0.3	12.5	13.1	105%
NMeFOSE	0.4	125.0	120.0	96%
NEtFOSE	0.4	125.0	123.3	99%
HFPO-DA	0.0	50.0	48.8	98%
ADONA	–	50.0	51.3	103%
PFMPA	0.0	25.0	26.2	105%
PFMBA	–	25.0	29.8	119%
NFDHA	–	25.0	21.3	85%
9Cl-PF3ONS	0.0	50.0	43.0	86%
11Cl-PF3OUdS	0.1	50.0	33.4	67%
PFEESA	–	25.0	24.7	99%
3:3 FTCA	–	50.0	79.4	159%
5:3 FTCA	1.2	250.0	329.1	132%
7:3 FTCA	0.7	250.0	289.4	116%

Conclusion

This application note presented an example of the experimental performance that can be obtained by following EPA Method 1633 for the analysis of 25 extracted internal standards (surrogates) and 40 target PFAS in aqueous samples. The method was verified using optimized solid-phase sample extraction and analysis using the 1290 Infinity II LC system coupled to the 6470 LC/TQ. Linearity was excellent for all analytes with R^2 values greater than 0.998 and RSEs less than 10%. Mid-concentration level precision and accuracy demonstrated strong performance with RSDs less than 9% and recoveries within typical EPA acceptance ranges. Initial method detection limits (MDL) were comparable to those in the method. The required one-minute retention time separation between bile salts (TDCA) and PFOS was achieved. Recoveries of both surrogate and target analytes in wastewater effluent spiked with all analytes were comparable to the spiked reagent water samples.

References

1. United States Environmental Protection Agency, Office of Water. Method 1633 Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous, Solid, Biosolids, and Tissue Samples by LC/MS/MS, **2024**. https://www.epa.gov/system/files/documents/2024-01/method-1633-final-for-web-posting.pdf (accessed April 29, 2024).
2. Hunt, *et al.* Analysis of Per- and Polyfluoroalkyl substances (PFAS) in Aqueous Samples Per EPA Method 1633, Agilent Bond Elut PFAS WAX SPE, *Agilent Technologies application note*, publication number 5994-5226EN, **2024**.

Additional resources

PFAS Water Testing. Get Ahead. Stay Ahead. Meet the Challenges of a Regulated Landscape – Start-to-Finish Workflows for PFAS Analysis. https://www.agilent.com/en/solutions/environmental/water-analysis/pfas-in-water

Appendix

Table 6. Agilent consumables and supplies for EPA Method 1633.

Description	Details	Part Number
PFC Delay Column	InfinityLab PFC Delay Column 4.6 x 30 mm	5062-8100
Guard Column	ZORBAX Eclipse Plus C18, 2.1 × 5 mm, 1.8 µm	821725-901
Analytical Column	ZORBAX Eclipse Plus C18, 2.1 × 100 mm; 1.8 µm	959758-902
Autosampler Vials	Vial, Screw, 2 mL, polypropylene, certified for PFAS, 100/pk	5191-8150
Autosampler Caps	Cap, 9 mm, screw, clear, thin membrane polypropylene/ silicone septa, certified for PFAS, 100/pk	5191-8151
Glass Wool	Glass wool, silane treated, 50 g	8500-1572
Centrifuge Tubes	Centrifuge tubes and caps, 15 mL, 50/pk	5610-2039
Carbon	Carbon SPE bulk sorbent, 25 g bottle	5982-4482
Syringes	5 mL disposable syringe, 100/pk	9301-6476
Nylon Filters	Agilent Captiva Premium Syringe Filter nylon, 25 mm, 0.2 µm, 100/pk	5190-5092

Table 7. dMRM transitions monitored.

Compound Group	Compound Name	Precursor Ion	Product Ion	RT (min)	Fragmentor	Collision Energy	Cell Accelerator Voltage
Acid	PFBA	213	168.9	3.5	60	8	2
Acid	PFPeA	263	219	4.5	72	4	2
Acid	PFHxA	313	268.9	5.2	70	8	2
Acid	PFHxA	313	119	5.2	70	18	2
Acid	PFHpA	362.9	319	5.7	72	4	2
Acid	PFHpA	362.9	169	5.7	72	14	2
Acid	PFOA	413	369	6.2	69	4	2
Acid	PFOA	413	169	6.2	69	12	2
Acid	PFNA	463	419	6.6	66	4	2
Acid	PFNA	463	219	6.6	66	17	2
Acid	PFDA	513	469	7.0	72	12	2
Acid	PFDA	513	219	7.0	72	20	2
Acid	PFUnA	563	519	7.5	100	12	2
Acid	PFUnA	563	269	7.5	100	20	2
Acid	PFDoA	613	569	7.9	100	8	2
Acid	PFDoA	613	319	7.9	100	20	2
Acid	PFTrDA	663	619	8.2	100	12	2
Acid	PFTrDA	663	169	8.2	100	32	2
Acid	PFTeDA	712.9	669	8.6	100	12	2
Acid	PFTeDA	712.9	169	8.6	100	32	2
Ether Sulfonic Acids	PFEESA	314.9	134.9	5.6	110	24	2
Ether Sulfonic Acids	PFEESA	314.9	83	5.6	124	20	5
Ether Sulfonic Acids	PFEESA	314.9	69	5.6	110	60	2
Ether Sulfonic Acids	9Cl-PF3ONS	530.9	350.9	7.6	145	28	2
Ether Sulfonic Acids	9Cl-PF3ONS	530.9	83	7.6	145	32	2
Ether Sulfonic Acids	11Cl-PF3OUdS	630.9	83	8.4	160	32	2

Compound Group	Compound Name	Precursor Ion	Product Ion	RT (min)	Fragmentor	Collision Energy	Cell Accelerator Voltage
Ether Sulfonic Acids	11Cl-PF3OUdS	630.9	450.9	8.4	165	32	2
Flurotelomer Carboxylic Acid	3-3 FTCA	241	177	4.2	74	4	3
Flurotelomer Carboxylic Acid	3-3 FTCA	241	117	4.2	74	44	3
Flurotelomer Carboxylic Acid	5-3 FTCA	341	237	5.6	84	12	3
Flurotelomer Carboxylic Acid	5-3 FTCA	341	217	5.6	84	24	3
Flurotelomer Carboxylic Acid	7-3 FTCA	441	337	6.6	76	12	3
Flurotelomer Carboxylic Acid	7-3 FTCA	441	317	6.6	76	24	3
FTS	4:2 FTS	327	306.9	5.0	125	20	2
FTS	4:2 FTS	327	80.9	5.0	125	36	2
FTS	6:2 FTS	427	406.8	6.0	125	24	2
FTS	6:2 FTS	427	80.9	6.0	125	40	2
FTS	8:2 FTS	527	507	6.8	200	30	4
FTS	8:2 FTS	527	80.9	6.8	170	40	2
ISTD	$^{13}C_3$-PFBA	216	171.9	3.5	65	8	2
ISTD	$^{13}C_2$-PFHxA	315	270	5.2	70	8	2
ISTD	$^{13}C_4$-PFOA	417	172	6.2	69	12	2
ISTD	$^{18}O_2$-PFHxS	403	83.9	6.4	100	49	2
ISTD	$^{13}C_5$-PFNA	468	423	6.6	66	4	2
ISTD	$^{13}C_2$-PFDA	515	470	7.0	81	4	2
ISTD	$^{13}C_4$-PFOS	503	80	7.3	148	54	2
ISTD	$^{13}C_4$-PFOS	502.9	98.9	7.3	180	48	2
Perfluorooctane Sulfonamide Ethanols	NMeFOSE	616	59	9.8	82	15	4
Perfluorooctane Sulfonamide Ethanols	NEtFOSE	630	59	10.1	124	45	4
Perfluorooctane Sulfonamides	PFOSA	497.9	478	8.6	150	36	3
Perfluorooctane Sulfonamides	PFOSA	497.9	78	8.6	150	36	3
Perfluorooctane Sulfonamides	PFOSA	497.9	48	8.6	150	110	3
Perfluorooctane Sulfonamides	NMeFOSA	512	219	9.9	156	28	5
Perfluorooctane Sulfonamides	NMeFOSA	512	169	9.9	156	32	5
Perfluorooctane Sulfonamides	NEtFOSA	526	269	10.3	160	28	5
Perfluorooctane Sulfonamides	NEtFOSA	526	219	10.3	160	28	5
Perfluorooctane Sulfonamides	NEtFOSA	526	169	10.3	160	28	5
Perfluorooctane Sulfonamidoacetic Acids	NMeFOSAA	570	482.9	7.1	150	16	2
Perfluorooctane Sulfonamidoacetic Acids	NMeFOSAA	570	419	7.1	150	20	2
Perfluorooctane Sulfonamidoacetic Acids	NEtFOSAA	584	526	7.3	100	20	2
Perfluorooctane Sulfonamidoacetic Acids	NEtFOSAA	584	419	7.3	100	20	2
Polyfluoroether Carboxylic Acids	PFMPA	229	84.9	4.0	60	12	2
Polyfluoroether Carboxylic Acids	PFMBA	279	235	4.8	80	1	5
Polyfluoroether Carboxylic Acids	PFMBA	279	84.9	4.8	70	12	2
Polyfluoroether Carboxylic Acids	NFDHA	295	201	5.1	75	5	2
Polyfluoroether Carboxylic Acids	NFDHA	295	85	5.1	120	32	5
Polyfluoroether Carboxylic Acids	NFDHA	201	85	5.1	70	15	5
Polyfluoroether Carboxylic Acids	HFPO-DA	285	185	5.4	50	20	5
Polyfluoroether Carboxylic Acids	HFPO-DA	285	169	5.4	50	4	5
Polyfluoroether Carboxylic Acids	ADONA	377	250.9	5.9	80	12	2
Polyfluoroether Carboxylic Acids	ADONA	377	85	5.9	80	36	2
Sulfonate	PFBS	298.9	98.9	5.3	100	29	2

Compound Group	Compound Name	Precursor Ion	Product Ion	RT (min)	Fragmentor	Collision Energy	Cell Accelerator Voltage
Sulfonate	PFBS	298.9	80	5.3	100	45	2
Sulfonate	PFPeS	348.9	98.9	5.9	135	40	2
Sulfonate	PFPeS	348.9	79.9	5.9	135	40	2
Sulfonate	PFHxS	398.9	99	6.4	100	45	2
Sulfonate	PFHxS	398.9	80	6.4	100	49	2
Sulfonate	PFHpS	448.9	98.7	6.9	100	44	2
Sulfonate	PFHpS	448.9	80	6.9	148	50	2
Sulfonate	PFOS	498.9	99	7.3	100	50	2
Sulfonate	PFOS	498.9	80	7.3	100	50	2
Sulfonate	PFNS	548.9	99	7.7	148	52	2
Sulfonate	PFNS	548.9	80	7.7	148	56	2
Sulfonate	PFDS	598.9	99	8.1	148	56	2
Sulfonate	PFDS	598.9	80	8.1	148	60	2
Sulfonate	PFDoS	698.9	99	8.8	156	62	2
Sulfonate	PFDoS	698.9	80	8.8	156	67	2
Surrogate	$^{13}C_4$-PFBA	217	172	3.5	60	8	2
Surrogate	$^{13}C_5$-PFPeA	268	223	4.5	60	8	2
Surrogate	$^{13}C_2$-4:2FTS	329	309	5.0	125	20	2
Surrogate	$^{13}C_2$-4:2FTS	329	81	5.0	150	32	2
Surrogate	$^{13}C_5$-PFHxA	318	273	5.2	70	8	2
Surrogate	$^{13}C_5$-PFHxA	318	120	5.2	72	24	2
Surrogate	$^{13}C_3$-PFBS	302	99	5.3	130	32	2
Surrogate	$^{13}C_3$-PFBS	302	80	5.3	130	44	2
Surrogate	$^{13}C_3$-HFPO-DA	287	185	5.4	64	20	5
Surrogate	$^{13}C_3$-HFPO-DA	287	169	5.4	64	4	5
Surrogate	$^{13}C_4$-PFHpA	367	322	5.7	72	4	2
Surrogate	$^{13}C_4$-PFHpA	367	169	5.7	72	16	2
Surrogate	$^{13}C_2$-6:2 FTS	429	409	6.0	125	24	2
Surrogate	$^{13}C_2$-6:2 FTS	429	81	6.0	150	40	2
Surrogate	$^{13}C_8$-PFOA	421	376	6.2	69	4	2
Surrogate	$^{13}C_8$-PFOA	421	172	6.2	72	20	2
Surrogate	$^{13}C_3$-PFHxS	402	99	6.4	156	44	2
Surrogate	$^{13}C_3$-PFHxS	402	80	6.4	100	45	2
Surrogate	$^{13}C_9$-PFNA	472	427	6.6	66	4	2
Surrogate	$^{13}C_9$-PFNA	472	223	6.6	72	16	2
Surrogate	$^{13}C_2$-8:2 FTS	529	509	6.8	170	28	2
Surrogate	$^{13}C_2$-8:2 FTS	529	81	6.8	200	52	4
Surrogate	$^{13}C_6$-PFDA	519	474	7.0	72	8	2
Surrogate	D3-NMeFOSAA	573.2	419	7.1	150	20	2
Surrogate	D5-NEtFOSAA	589.2	419	7.2	100	20	2
Surrogate	$^{13}C_8$-PFOS	507	99	7.3	148	52	2
Surrogate	$^{13}C_8$-PFOS	507	80	7.3	100	50	2
Surrogate	$^{13}C_7$-PFUnA	570	525	7.5	100	8	2
Surrogate	$^{13}C_2$-PFDoA	615	570	7.9	90	12	2
Surrogate	$^{13}C_2$-PFTeDA	715	670	8.6	90	12	2
Surrogate	$^{13}C_8$-PFOSA	506	78	8.6	150	36	3

Compound Group	Compound Name	Precursor Ion	Product Ion	RT (min)	Fragmentor	Collision Energy	Cell Accelerator Voltage
Surrogate	D7-NMeFOSE	623.2	59	9.8	82	15	4
Surrogate	D3-NMeFOSA	515	219	9.9	156	28	5
Surrogate	D9-NEtFOSE	639.2	59	10.1	124	45	4
Surrogate	D5-NEtFOSA	531	219	10.2	160	28	5
TDCA	TDCA	498.3	79.9	6.0	165	32	2

www.agilent.com

DE62533826

This information is subject to change without notice.

Printed in the USA, July 9, 2024
5994-4926EN

Agilent
Trusted Answers