

Analysis of Per- and Polyfluoroalkyl Substances (PFAS) Specified in EPA M8327 using the LCMS-8050 Triple Quadrupole Mass Spectrometer

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■ Abstract

The Environmental Protection Agency (EPA) has recently published draft SW-846 Method 8327 for the analysis of PFAS in groundwater, surface water, and wastewater. No other EPA method for PFAS analysis in complex matrices was available; hence, this method in its final version will provide a tool for monitoring selected PFAS in non-potable waters. This application note demonstrates that the LCMS-8050 meets and exceeds the Quality Assurance and Quality Control criteria specified in the method. All analytes were reliably quantitated at or less than 5 ppt. Ultimately, this work provides a fast and robust solution for addressing the challenges in the quantitation of low levels of PFAS in non-potable waters.

■ Background

Per- and Polyfluorinated Alkyl Substances (PFAS) are a group of anthropogenic chemicals widely used in consumer products (e.g. food packaging materials and non-stick coatings) and industrial applications (firefighting foams, polymers/plastics manufacturing). Their unique properties, such as being highly stable and resistant to degradation¹, together with their ubiquitous use has resulted in the accumulation of PFAS in the environment.

The PFAS family encompasses over 4,000 chemicals, with the commonality of having a per- or poly-fluorinated carbon backbone compounds. Due to their potential deleterious effects on humans and ecosystems, PFOA and PFOS are no longer manufactured in the US; this has resulted in the introduction of replacement chemicals. There is a need of robust and fast analytical methods to ensure accurate quantitation of low levels (in low ng/L range) of legacy and replacement PFAS entering the environment and there are concerns about their effects on humans and ecosystems as well as the compounds ability to repel oil and water.

Research into the adverse health effects²⁻⁶ of PFAS in humans is ongoing. Many studies have linked PFOA and PFOS to reproductive damage, liver and kidney damage, and weakened immune systems. PFAS exposure has also been linked to elevated cholesterol levels.

This application note provides a fast and robust solution based on the use of Shimadzu LCMS-8050 for all analytes listed in EPA Method 8327. Results demonstrate that the instrument's performance exceeds the requirements outlined in the draft EPA method. Most importantly, the results confirm that laboratories currently analyzing samples by ASTM Method D7979⁷⁻⁸ using Ultra-fast LC-MS/MS (UFMS™) Analysis of PFAS in environmental samples can easily update their workflow to implement EPA Method 8327.

Keywords: Per- and Polyfluorinated Alkyl Substances, PFAS, Perfluorinated Compounds, PFCs, PFOA, PFOS, Persistent Organic Pollutants, POPs, Triple Quad, Wastewater, Ground Water, Surface Water, EPA Method 8327, ASTM D7979

■ Analyte List

EPA Method 8327 analyzes 24 target PFAS compounds and 19 surrogates in reagent, ground, surface, and wastewater. Target compounds and their respective acronyms, surrogate compounds, and their chemical classes are listed in Table 1. For the remainder of this application note, refer to the acronyms in Table 1.

Table 1: Target analytes, surrogates, acronyms and CAS # included in this method

Analyte	Acronym	CAS #	Surrogates
Sulfonic acids			
Perfluorobutyl sulfonic acid	PFBS	29420-49-3	13C3-PFBS
Perfluorohexyl sulfonic acid	PFHxS	3871-99-6	13C3-PFHxS
Perfluorooctyl sulfonic acid	PFOS	1763-23-1	13C8-PFOS
1H,1H, 2H, 2H-perfluorohexane sulfonic acid	4:2 FTS	757124-72-4	13C2-4:2 FTS
1H, 1H, 2H, 2H-perfluorooctane sulfonic acid	6:2 FTS	27619-97-2	13C2-6:2 FTS
1H, 1H, 2H, 2H-perfluorodecane sulfonic acid	8:2 FTS	39108-34-4	13C2-8:2 FTS
Perfluoro-1-pentanesulfonic acid	L-PFPeS	706-91-4	-
Perfluoro-1-heptanesulfonic acid	L-PFHpS	375-92-8	-
Perfluoro-1-nonanesulfonic acid	L-PFNS	68259-12-1	-
Perfluoro-1-decanesulfonic acid	L-PFDS	2806-15-7	-
Carboxylic acids			
Perfluorobutanoic acid	PFBA	375-22-4	13C4-PFBA
Perfluoropentanoic acid	PFPeA	2706-90-3	13C5-PFPeA
Perfluorohexanoic acid	PFHxA	307-24-4	13C5-PFHxA
Perfluoroheptanoic acid	PFHpA	375-85-9	13C4-PFHpA
Perfluorooctanoic acid	PFOA	335-67-1	13C8-PFOA
Perfluorononanoic acid	PFNA	375-95-1	13C9-PFNA
Perfluorodecanoic acid	PFDA	335-76-2	13C6-PFDA
Perfluoroundecanoic acid	PFUnA	2058-94-8	13C7-PFUnA
Perfluorododecanoic acid	PFDoA	307-55-1	13C2-PFDoA
Perfluorotridecanoic acid	PFTriA	72629-94-8	-
Perfluorotetradecanoic acid	PFTreA	376-06-7	13C2-PFTreA
Sulfonamides and sulfonamidoacetic acids			
N-ethylperfluoro-1-octanesulfonamidoacetic acid	N-EtFOSAA	2991-50-6	D3-N-EtFOSAA
N-methylperfluoro-1-octanesulfonamidoacetic acid	N-MeFOSAA	2355-31-9	D3-N-MeFOSAA
Perfluoro-1-octanesulfonamide	FOSA	754-91-6	13C8-PFOSA

■ Method

This application news describes and demonstrates the use and performance of the Shimadzu LCMS-8050 for the analysis of 43 PFAS, 24 targets and 19 surrogates, in reagent, ground, surface and wastewater matrices as outlined in draft EPA M8327 (as of September 2019). EPA provided a set of supplies including 15 mL polypropylene (PP) tubes, analytical column, delay column, PFAS precision and recovery standard (Wellington), labeled PFAS extraction standard (Wellington), certified amber glass 2 ml vials, PP septumless caps for 2 ml vials, GXF/GHP syringe filters membrane 0.2 µm filters and 10 ml metal luer-lock all glass syringe.

An equivalent to Shimadzu Shim-pack GIST Phenyl-Hexyl, 2.1×100 mm and 3.0 µm particle size analytical column was used to conduct the analysis for all PFAS compounds (Shimadzu part no. 227-30713-03) along with a Shimadzu Shim-pack XR-ODS 50mm x 3.0mm x 2.2 µm as delay column (Shimadzu part no 228-41606-92). Multiple Reaction Monitoring (MRM) transitions were optimized using Flow Injection Analysis (FIA) for all compounds.

Mobile Phase A consisted of 20 mM Ammonium acetate in 95:5 H₂O: ACN. Mobile Phase B consisted of 10 mM ammonium acetate in 95:5 ACN: H₂O. A 30 µL injection volume was used for all calibration levels. A 0.3 mL/min flow rate was used. Chromatography was adjusted to obtain maximum resolution between peaks in the shortest time possible with minimum co-elution of isomers. Overall runtime for each injection was 21 minutes, including re-equilibration for both the delay and the analytical column. The total run time of 21 minutes includes a final wash out with concentrated acetonitrile to flush the column, remove background residuals contaminants and restore column performance before starting the next run. The method could easily be modified to include isotopic dilution or internal calibration if needed for quantifying the concentrations.

The LC/MS/MS analysis was performed using a Shimadzu Nexera UHPLC system coupled with LCMS-8050 triple quadrupole mass spectrometer. An injection volume of 30 µL was used in this study. A detailed description of the LC/MS/MS parameters is included in Table 2.

Table 2: Chromatography and mass spectrometer conditions

Parameter	Value	
LCMS	Shimadzu LCMS-8050	
Analytical Column	Shim-pack GIST Phenyl-Hexyl (2.1 mm ID. x 100 mm L., 3 µm) Part No 227-30713-03	
Solvent Delay Column	Shim-pack XR-ODS (3 mm ID. x 50 mm L., 2.2 µm) Part No. 228-41606-92	
Column Oven Temperature	40 °	
Injection Volume	30 µL	
Mobile Phase	A: 20 mmol Ammonium Acetate in 5 % (v/v) Acetonitrile in reagent water B: 10 mmol Ammonium Acetate in 95 % (v/v) Acetonitrile in reagent water	
Gradient Flow rate	0.3 mL/ Min	
Gradient	Time (minutes)	% B
	0	0
	1	20
	6	50
	14	100
	17	100
	18	0
	21	0
Run time	21 minutes	
Nebulizing gas flow	5 L/min	
Heating gas flow	15 L/Min	
Interface temperature	300 °C	
Desolvation Line temperature	100 °C	
Heat Block temperature	200 °C	
Drying gas flow	5 L /min	
Acquisition cycle time	21 min	
Total MRMs	66	

Fluorotelomer acids, observed as $[M-H]^-$ and $[M-HF-H]^-$ can result in an ion with the same m/z as the unsaturated fluorotelomer acid. Even under optimized chromatography, these compounds have near identical retention times. The lower ESI heater temperature reduces HF loss and minimizes false identification of fluorotelomer acids. Temperature conditions may vary depending on the type of applications performed⁹.

All compound parameters, including precursor ion, product ion, and collision energies were optimized using FIA, bypassing the analytical column using Lab Solutions software. There are at least two MRM transitions for most of the analytes that are listed in Table 3.

Table 3: MRM transitions, retention times and collision energies

Component	Retention Time (minutes)	Transition (m/z)	Collision energy (V)
PFBA	3.341	213 > 169	9
MPFBA	3.341	217 > 172	9
PFPeA	3.941	263 > 219	8
M5PFPeA	3.940	268 > 223	8
4-2 FTS	4.444	327 > 307	18
		327 > 81	35
M4-2 FTS	4.442	329 > 309	20
PFHxA	4.683	313 > 269	9
		313 > 119	21
M5PFHxA	4.680	318 > 273	11
PFBS	4.709	299 > 80	30
		299 > 99	28
M3PFBS	4.813	302 > 80	34
PFHpA	5.401	363 > 319	9
		363 > 169	16
M4PFHpA	5.400	367 > 322	10
PFPeS	5.606	349 > 80	42
		349 > 99	30

6-2 FTS	5.797	427 > 407 427 >81	23 39
M6-2 FTS	5.799	429 >409	22
PFOA	6.048	413 > 369 413 >169	10 17
M8PFOA	6.051	421 > 376	10
PFHxS	6.305	399 > 80 399 >99	43 22
M3PFHxS	6.306	402 > 80 403 >84	49 49
PFNA	6.642	463 > 419 463 >219	11 16
M9PFNA	6.641	472 > 427	12
8-2 FTS	6.927	527 > 507 527 >81	26 49
M8-2 FTS	6.928	529 > 509 527 >81	26 49
PFHpS	6.928	449 > 80 449 >99	51 37
N-MeFOSAA	7.254	570 > 419 570 >483	21 16
d3M N-MeFOSAA	7.243	573 > 419	20
PFDA	7.189	513 > 468.9 413 >219	11 17
M6PFDA	7.188	519 > 474	11
N-EtFOSAA	7.469	584 > 419 584 >483	20 16
M N-EtFOSAA	7.463	589 > 419	21
PFOS	7.483	499 > 80 499 >99	54 38
M8PHOS	7.484	507 > 80	55
PFUdA	7.697	563 > 519 563 >269	12 16
M7PFUdA	7.695	570 > 525	12
PFNS	8.009	549 > 80 549 >99	54 44
PFDoA	8.181	613 > 569 613 >169	12 21
MPFDoA	8.179	615 > 570	11
FOSA	8.498	498 > 78	43
M8FOSA	8.498	506 > 78	48
PFDS	8.523	599 > 80 599 >99	55 50
PFTriA	8.662	663 > 619 663 >169	12 27
PFTeDA	9.155	713 > 669 713 >169	13 27
M2PFTeDA	9.130	715 > 670	15

Calibration Standards

Standards available from Wellington Laboratories were used for these studies (Catalog no. PFAC-24PAR and MPFAC-24ES). These standards were then diluted to working standards as outlined in Section 7.4 of EPA Method 8327 using 95:5 acetonitrile:water as the diluent. The working standards were used to create a calibration curve ranging from 5-200 ppt with the injection solvent consisting of 50:50 water:methanol with 0.1% acetic acid in order to match the injection solvent for the extracted samples. Filtration was not performed on the calibration standards

Sample Preparation

EPA Method 8327 was tested using reagent water, surface water, ground water, and wastewater as sample matrices. This report outlines data collected with representative chromatograms and tables for each matrix tested. Each sample was diluted 50:50 with MeOH and 0.1% acetic acid, spiked with isotopically labeled surrogates and vortexed for 2 min. The samples were then filtered through /0.2 µm syringe filters and analyzed by LC/MS/MS.

■ Results and Discussion

It is known that PFAS can be present in reagents, glassware, pipettes, tubing, degassers and other parts from the LC-MS/MS instruments. PFAS contamination coming from the LC system is eliminated using a delay column placed between the reagents and the sample valve. This separates PFAS in the sample from the PFAS in the LC system. All supplies used to conduct the study were free from PFAS contamination. To monitor the lack of contamination two blanks were injected at the beginning of each batch: system null injection (air injection, shown in Figure 1) and reagent blank (0.1% acetic acid in high purity water:methanol (50:50), shown in Figure 2). Data displayed in Figures 1 and 2 demonstrates the absence of PFAS in the instrument and the materials used for analysis, respectively.

Calibration was performed for all PFAS targets using a nine-point calibration curve, ranging from 5 ng/L - 200 ng/L. The linearity of the curve was determined using a 1/x weighting factor and not forcing through zero. Excellent linearity was obtained with correlation coefficients (r^2) greater than 0.99 for all analytes or transitions. Calibration residuals of each standards were within $\pm 30\%$. Figure 3 shows a total ion chromatogram and MRMs from a 5 ng/L standard; this figure demonstrates the separation and peak shape of targets at the lowest concentration included in the calibration curve. Figure 4 shows a chromatogram of a mid-level standard at 80 ng/L for all PFAS targets and surrogate compounds included in draft EPA method 8327 and confirms that peak shape is maintained at higher concentrations.

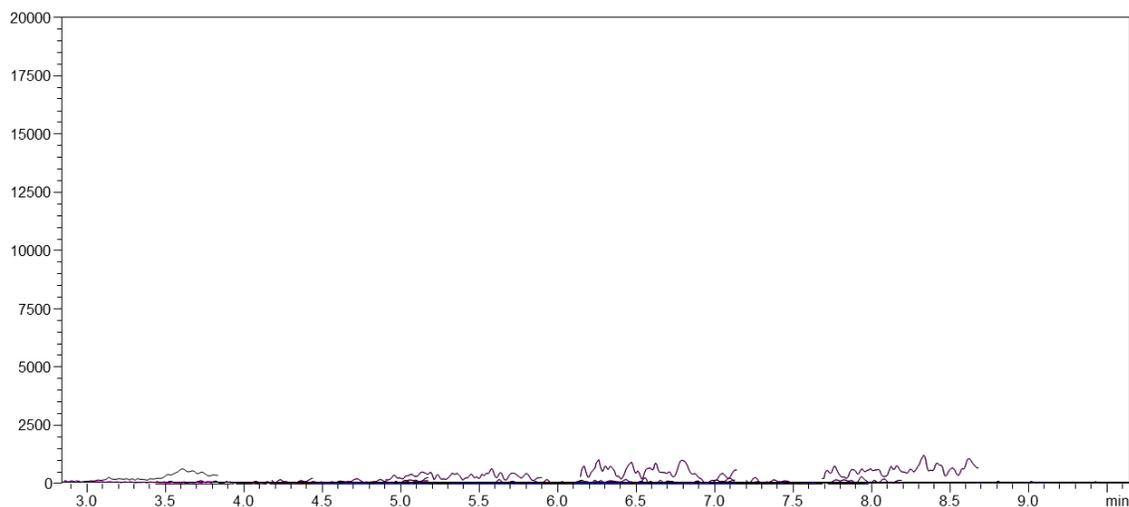


Figure 1: TIC Chromatogram of a Null Blank

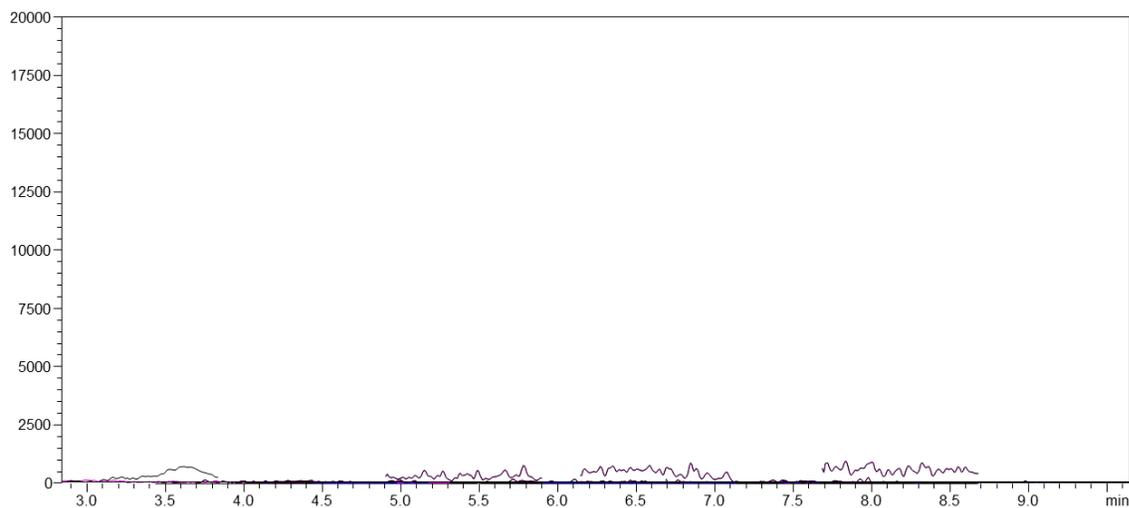


Figure 2: TIC Chromatogram of a reagent blank in 50:50 MeOH: H2O with 0.1% acetic acid

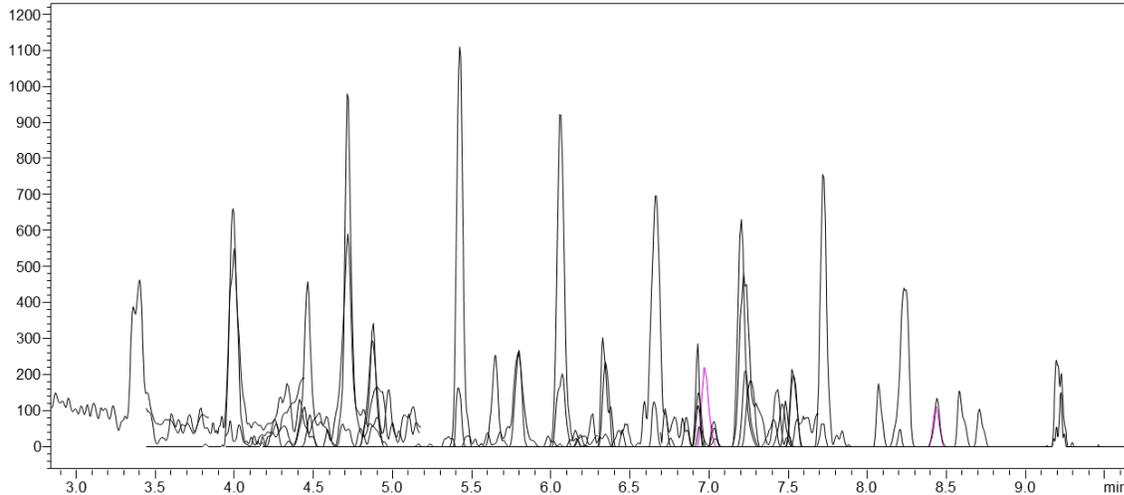


Figure 3: TIC (black) chromatograms and MRM transitions (other colors) of all PFAS in EPA Method 8327 at the low-level calibrator, 5 ppt

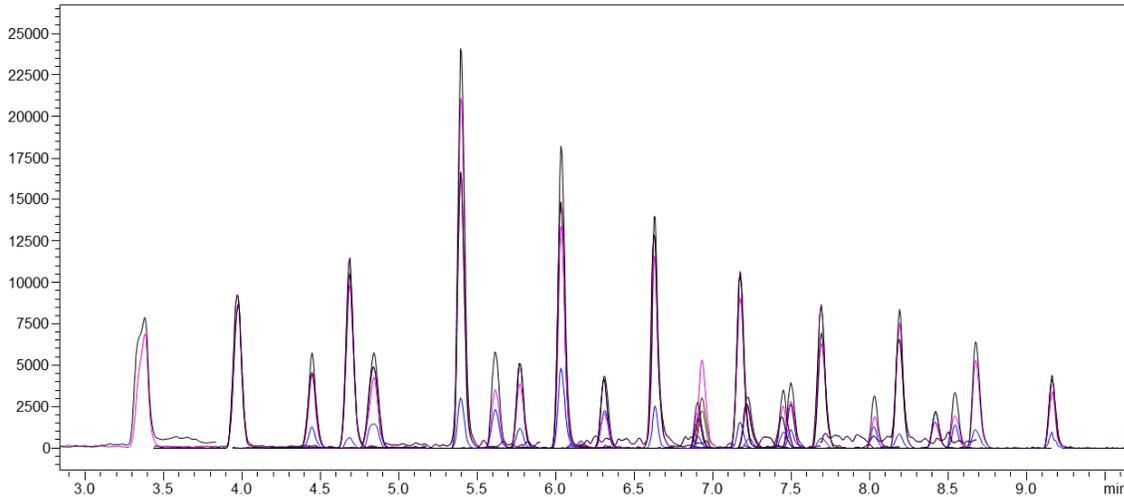


Figure 4 TIC (black) chromatograms and MRM transitions (other colors) of all PFAS in EPA Method 8327 at the mid-level, 80ppt calibrator

Figure 5 shows an extracted ion chromatogram of representative peak at 5 ng/L and calibration curves for PFHxS, PFOS and PFTreA. Table 4 lists the calculated concentrations, percent recovery for all targets in EPA Method 8327 at representative low, mid and high-level concentrations. All percent recoveries were within the limits established as acceptable in draft method EPA 8327 (50%-150% for the lowest calibration standard and 70%-130% for the remaining ones). Signal to Noise ratio for each target compound at 5 ng/L is also included in Table 4. All compounds except PFHxS presented S/N larger than 3 these results suggest that for most of the compounds lower sensitivity could be achieved.

Figure 6 shows the chromatogram for 24 PFAS compounds spiked at 60 ppt in various matrices, including reagent water, ground water, surface water, and wastewater. Results show that despite the differences in the sample composition and presence of potential interferences, the separation and peak shape is maintained in all samples types analyzed.

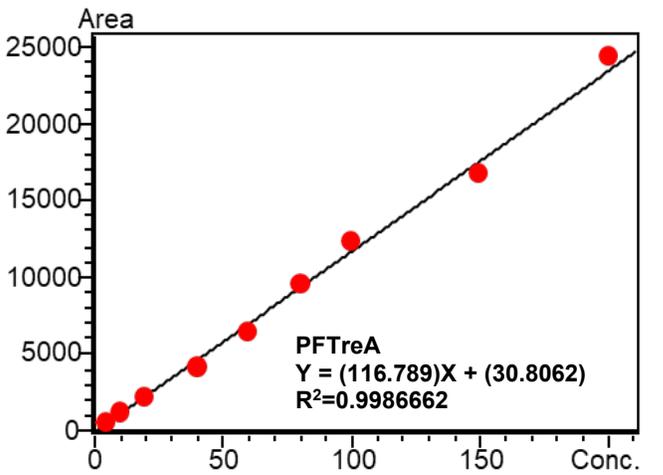
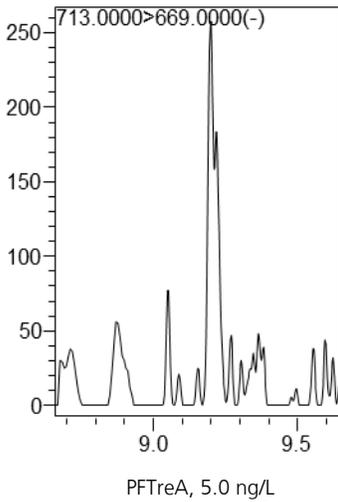
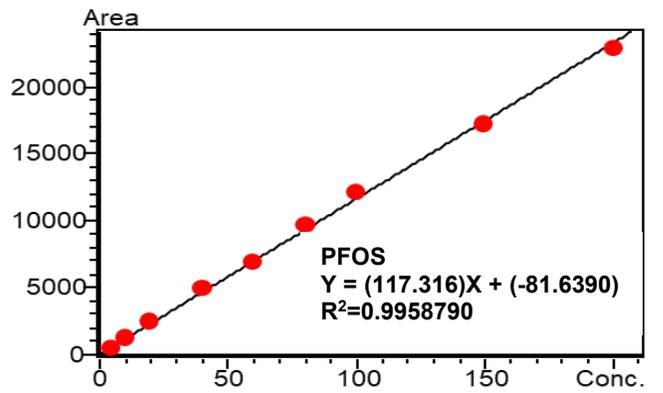
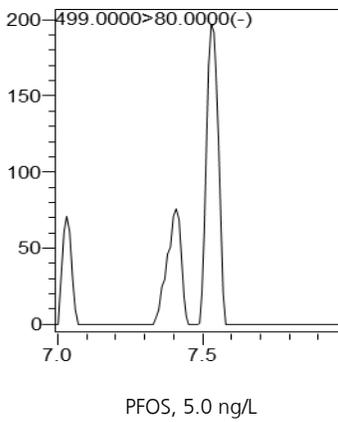
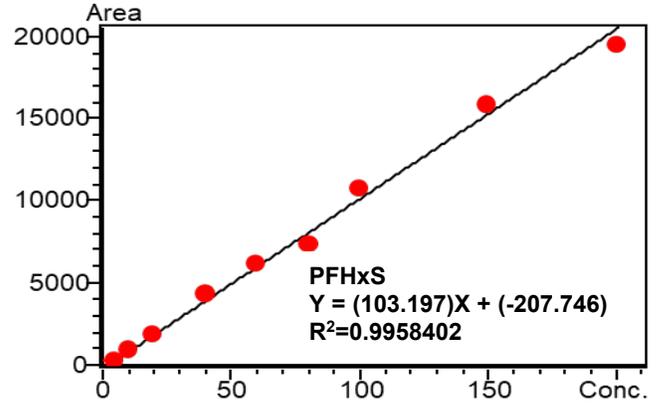
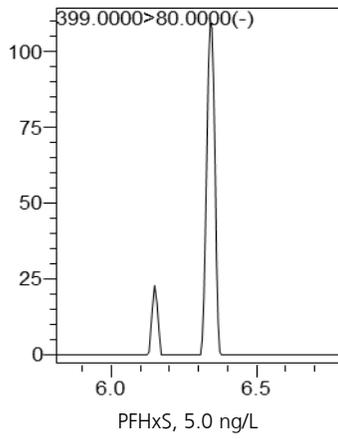
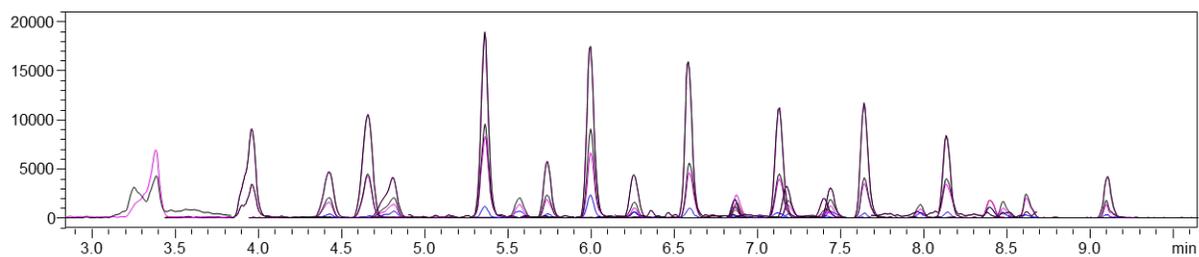
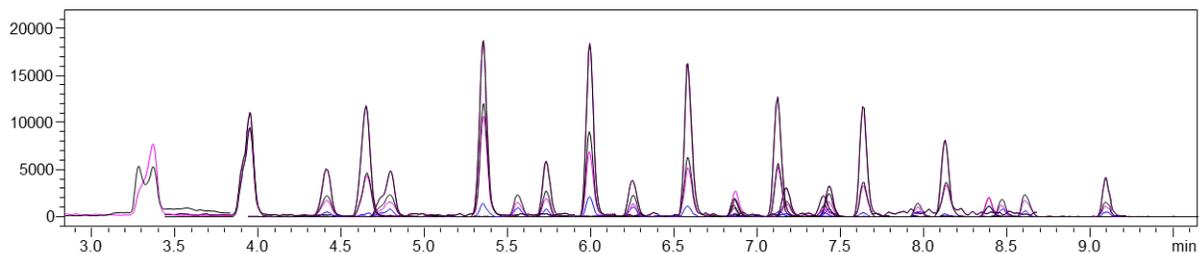


Figure 5: Representative Chromatograms and Calibration curves for compounds listed in EPA Method 8327

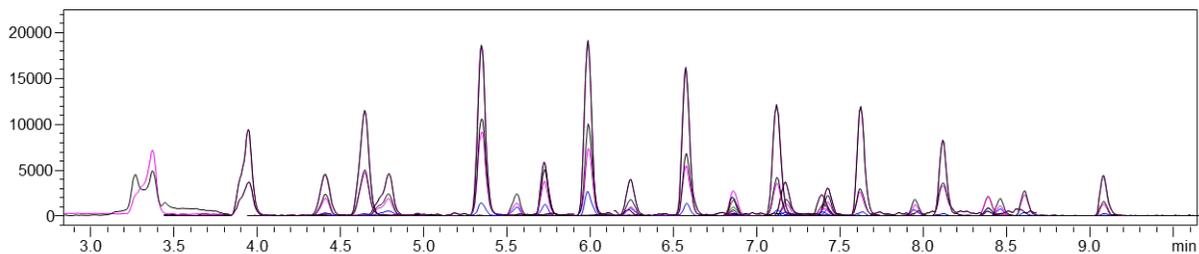
A. Reagent Water



B. Ground Water



C. Surface Water



D. Waste Water

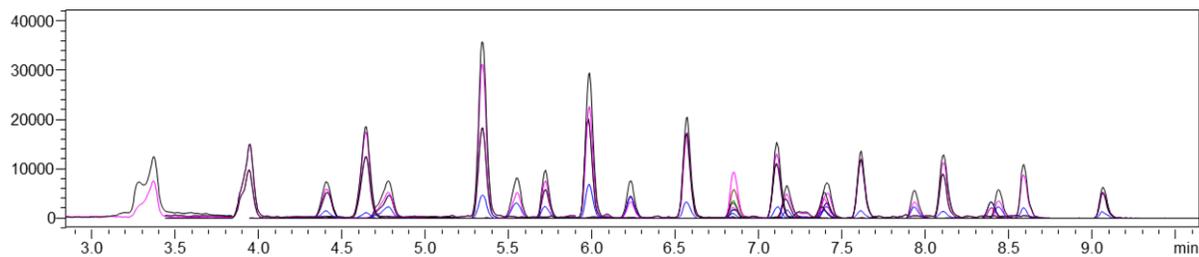


Figure 6: Chromatogram (TIC and MRMs) of 24 PFAS Compounds spiked at the 60 ng/L in: A) Reagent Water; B) Ground Water; C) Surface Water, and D) Waste Water

Table 4: Calculated concentrations for the low, mid, and high-level standards for all targets in EPA Method 8327.

Compound	RT (min)	Conc	5 ppt		40 ppt		200 ppt	
			% Recoveries	Signal/noise (S/N) (*)	Conc	% Recoveries	Conc	% Recoveries
PFBA	3.382	4.48	90	3.28	42.37	106	196.7	98
M4PFBA	3.378	4.65	93	72.36	40.14	100	200.1	100
PFPeA	3.897	5.20	104	21.57	41.49	104	200.8	100
M5PFPeA	3.892	5.09	102	268.79	40.34	101	202.3	101
4-2 FTS	4.333	4.56	91	212.65	41.08	103	199.8	100
M2-4-2 FTS	4.319	4.82	96	71.11	41.48	104	200.8	100
PFHxA	4.544	4.95	99	44.95	41.10	103	198.3	99
M5PFHxA	4.542	4.99	100	830.68	40.57	101	198.5	99
PFBS	4.676	4.25	85	9.21	38.96	97	195.2	98
M3PFBS	4.674	5.15	103	172.98	39.32	98	202.2	101
PFHpA	5.219	4.99	100	37.17	39.01	98	196.1	98
M4PFHpA	5.217	4.93	99	1247.7	38.68	97	199.6	100
PFPeS	5.399	5.31	106	196.02	41.15	103	199.6	100
6-2 FTS	5.586	4.25	85	75.54	37.33	93	183.1	92
M2-6-2 FTS	5.591	4.94	99	61.36	39.19	98	205.0	103
PFOA	5.826	4.61	92	46.56	40.05	100	198.7	99
M8PFOA	5.827	4.50	90	611.9	41.73	104	195.5	98
PFHxS	6.062	5.69	114	(INF)	41.34	103	195.3	98
M3PFHxS	6.064	5.08	102	(INF)	41.46	104	204.1	102
PFNA	6.401	3.83	77	23.64	38.10	95	198.9	100
M9PFNA	6.397	5.13	103	292.26	39.58	99	195.4	98
8-2 FTS	6.681	4.04	81	(INF)	33.29	83	200.1	100
M2-8-2 FTS	6.673	4.92	98	31.79	35.90	90	198.6	99
PFHpS	6.663	4.35	87	(INF)	41.09	103	197.8	99
N-MeFOSAA	7.005	5.30	106	(INF)	39.93	100	208.6	104
d3-NMeFOSAA	7.001	5.98	120	(INF)	39.33	98	197.8	99
PFDA	6.93	5.45	109	64.37	40.68	102	201.1	101
M6PFDA	6.927	5.02	100	596.91	39.27	98	201.5	101
N-EtFOSAA	7.221	5.67	113	14.63	38.42	96	202.8	101
d5-NEtFOSAA	7.221	5.45	109	(INF)	44.72	112	200.8	100
PFOS	7.204	5.39	108	(INF)	34.56	86	196.8	98
M8PFOS	7.201	4.71	94	(INF)	36.86	92	195.4	98
PFUnA	7.426	5.42	108	21.82	41.21	103	197.1	99
M7PFUnA	7.423	5.34	107	545.68	43.51	109	203.8	102
PFNS	7.705	4.94	99	(INF)	44.30	111	198.2	99
PFDoA	7.893	5.14	103	54.66	37.82	95	205.8	103
M2PFDoA	7.889	5.11	102	(INF)	39.36	98	202.2	101
FOSA	8.207	4.95	99	(INF)	41.83	105	200.8	100
M8FOSA	8.215	4.94	99	1663.83	41.12	103	201.9	101
PFDS	8.188	4.94	99	(INF)	41.55	104	200.1	100
PFTriA	8.359	4.40	88	43.58	42.18	105	198.1	99
PFTreA	8.816	4.66	93	21.34	39.44	99	199.8	100
M2PFTreA	8.82	4.48	99	1703.08	37.43	94	198.0	99

(*) INF: S/N value when background noise is zero for a compound.

Table 5 outlines the Accuracy (spike %recovery) and precision (%RSD) of targets and surrogates spiked at 80 ng/L in reagent water. The mean recovery for all compounds were within 70 to 130% and the precision (%RSD) were \leq 20%, well within the QA criteria outlined in drafted EPA method 8327.

Tables 6-9 outline the surrogate percent recoveries and precision (%RSD) spiked at 160 ng/L in, reagent water, ground water, surface water and wastewater samples. Surrogate recoveries for all PFASs tested were within 70 to 130% as required by the method acceptance criteria and the precision (RSD%) were \leq 20%.

Table 5: Accuracy (spike %recovery) and precision (%RSD) 24 PFASs and 19 mass-labeled surrogates at 80 ng/L, spiked in reagent water.

Component	#1	#2	#3	#4	Average Concentration (ng/L)	%Average Recovery	%RSD
PFBA	81.5	83.9	84.1	83.1	83.1	103.9	1.4
MPFBA	79.3	81.4	81.3	81.3	80.8	101.0	1.3
PFPeA	78.2	78.3	81.5	82.8	80.2	100.3	2.8
M5PFPeA	77.9	77.8	80.6	80.6	79.2	99.0	2.0
4-2 FTS	78.5	84.1	81.8	84.1	82.1	102.6	3.2
M4-2 FTS	78.5	82.0	78.3	83.1	80.5	100.6	3.1
PFHxA	80.0	80.3	79.9	81.7	80.5	100.6	1.1
M5PFHxA	80.3	82.3	80.9	81.0	81.1	101.4	1.1
PFBS	78.0	81.0	79.2	83.6	80.5	100.6	3.0
M3PFBS	77.7	81.0	81.2	81.8	80.4	100.5	2.3
PFHpA	81.1	81.8	81.6	82.4	81.7	102.1	0.6
M4PFHpA	80.8	81.3	80.5	78.0	80.1	100.2	1.8
PFPeS	78.2	78.9	79.7	82.4	79.8	99.8	2.3
6-2 FTS	80.3	90.8	90.1	80.5	85.4	106.8	6.7
M6-2 FTS	79.0	86.3	79.7	75.9	80.2	100.3	5.5
PFOA	80.7	80.9	80.0	82.8	81.1	101.4	1.4
M8PFOA	79.0	82.4	84.3	83.9	82.4	103.0	2.8
PFHxS	71.6	74.3	75.6	76.1	74.4	93.0	2.7
M3PFHxS	78.4	78.3	81.9	79.6	79.5	99.4	2.1
PFNA	78.9	74.8	84.4	79.5	79.4	99.3	4.9
M9PFNA	79.0	79.8	79.8	77.7	79.1	98.9	1.3
8-2 FTS	82.3	75.3	88.1	68.6	78.6	98.3	10.7
M8-2 FTS	87.0	80.1	81.8	84.4	83.3	104.1	3.6
PFHpS	81.3	81.0	79.2	79.8	80.3	100.4	1.26
N-MeFOSAA	79.5	76.7	94.3	80.7	82.8	103.5	9.5
d3M N- MeFOSAA	74.5	83.1	83.5	78.3	79.9	99.8	5.4
PFDA	81.3	80.4	79.1	84.5	81.3	101.7	2.8
M6PFDA	81.1	78.6	81.7	83.2	81.2	101.4	2.4
N-EtFOSAA	66.8	78.1	83.0	69.0	74.2	92.8	10.2
M N-EtFOSAA	74.3	69.6	75.1	82.0	75.3	94.1	6.7
PFOS	74.2	74.4	71.5	80.9	75.2	94.0	5.3
M8PHOS	77.8	78.7	73.9	79.7	77.5	96.9	3.3
PFUdA	77.5	81.6	87.3	79.1	81.4	101.7	5.3
M7PFUdA	75.8	80.1	82.7	85.4	81.0	101.3	5.1
PFNS	77.0	82.5	95.6	85.4	85.1	106.4	9.2
PFDoA	74.4	79.2	80.5	78.8	78.2	97.8	3.4
MPFDoA	75.8	78.1	79.3	78.9	78.0	97.6	2.0
FOSA	75.4	80.9	85.6	81.8	80.9	101.2	5.2
M8FOSA	80.0	83.1	81.6	83.0	81.9	102.4	1.7
PFDS	78.1	83.2	78.6	82.7	80.7	100.8	3.3
PFTriA	76.0	79.4	78.9	82.7	79.2	99.1	3.4
PFTeDA	71.3	85.8	83.9	78.8	80.0	100.0	8.1
M2PFTeDA	67.1	76.7	78.5	82.3	76.2	95.2	8.5

Table 6: Ground Water - Surrogates Spike Recoveries: Accuracy (%recovery) and precision (%RSD) at 160 ng/L.

Sample ID	160 ng/L #1	160 ng/L #2	160 ng/L #3	160 ng/L #4	%Average Recovery (ng/L)	%RSD
d3-NMeFOSAA	182.7	170.8	219.4	173.5	116.7	12.0
d5-NEtFOSAA	165.1	188.6	174.0	169.9	109.0	5.8
M2-4-2 FTS	144.6	163.7	153.0	146.9	95.0	5.6
M2-6-2 FTS	164.9	157.6	168.4	141.3	98.8	7.6
M2-8-2 FTS	152.7	194.6	177.2	172.0	108.9	9.9
M2PFDoA	185.9	197.6	215.0	187.3	122.8	6.8
M2PFTreA	219.0	223.5	232.1	208.4	138.0	4.5
M3PFBS	174.0	175.5	180.2	175.6	110.2	1.5
M3PFHxS	184.5	202.9	196.5	176.1	118.8	6.3
M4PFBA	181.0	195.4	189.1	186.9	117.6	3.2
M4PFHpA	180.3	188.0	190.1	180.2	115.4	2.8
M5PFHxA	186.2	199.9	193.6	168.7	117.0	7.2
M5PFPeA	182.4	192.4	193.8	182.1	117.3	3.4
M6PFDA	182.5	179.5	194.2	176.7	114.6	4.2
M7PFUnA	185.4	191.9	204.3	196.0	121.5	4.1
M8FOSA	193.4	194.6	215.3	184.7	123.1	6.6
M8PFOA	182.2	187.9	188.9	179.7	115.5	2.4
M8PFOS	184.2	188.9	198.3	185.5	118.3	3.4
M9PFNA	173.9	186.0	195.7	182.8	115.4	4.9

Table 7: Reagent Water -Surrogates Spike Recoveries: Accuracy (%recovery) and precision (%RSD) at 160 ng/L.

Sample ID	160 ng/L #1	160 ng/L #2	160 ng/L #3	160 ng/L #4	%Average Recovery (ng/L)	%RSD
d3-NMeFOSAA	152.5	158.2	152.3	155.7	96.7	1.8
d5-NEtFOSAA	145.8	144.1	139.2	153.2	91.0	4.0
M2-4-2 FTS	129.5	146.5	136.2	130.7	84.8	5.7
M2-6-2 FTS	139.5	145.2	136.5	131.2	86.3	4.2
M2-8-2 FTS	124.3	139.7	156.5	145.1	88.4	9.5
M2PFDoA	149.2	152.6	152.2	148.4	94.2	1.4
M2PFTreA	143.2	140.9	148.6	136.8	89.0	3.5
M3PFBS	133.1	152.9	138.7	141.2	88.4	5.9
M3PFHxS	137.6	146.1	149.4	142.9	90.0	3.5
M4PFBA	140.2	126.2	140.7	138.7	85.3	5.0
M4PFHpA	147.8	154.2	152.1	153.3	94.9	1.9
M5PFHxA	151.3	152.2	154.5	146.5	94.5	2.2
M5PFPeA	145.6	152.1	147.4	148.7	92.8	1.8
M6PFDA	150.2	151.3	148.8	154.1	94.5	1.5
M7PFUnA	146.0	149.6	150.3	144.7	92.3	1.8
M8FOSA	143.3	171.0	149.2	134.3	93.4	10.4
M8PFOA	145.7	157.8	153.7	145.5	94.2	4.0
M8PFOS	139.2	141.6	140.6	140.9	87.9	0.7
M9PFNA	153.3	149.2	156.6	157.5	96.4	2.4

Table 8: Surface Water -Surrogates Spike Recoveries: Accuracy (%recovery) and precision (%RSD) at 160 ng/L.

Sample ID	160 ng/L #1	160 ng/L #2	160 ng/L #3	160 ng/L #4	%Average Recovery (ng/L)	%RSD
d3-NMeFOSAA	159.9	134.1	139.7	132.6	88.5	8.9
d5-NEtFOSAA	133.1	144.2	140.6	111.3	82.7	11.1
M2-4-2 FTS	149.9	134.2	122.9	132.3	84.3	8.3
M2-6-2 FTS	141.3	124.5	134.4	132.6	83.3	5.2
M2-8-2 FTS	143.2	131.1	128.0	116.8	81.1	8.4
M2PFDoA	157.3	146.4	146.2	137.8	91.8	5.4
M2PFTreA	155.9	138.4	135.4	137.4	88.6	6.7
M3PFBS	153.7	136.2	143.5	132.2	88.4	6.7
M3PFHxS	153.5	128.0	143.6	131.4	87.0	8.4
M4PFBA	155.8	140.6	141.6	132.9	89.2	6.7
M4PFHpA	155.9	139.4	140.2	130.7	88.5	7.4
M5PFHxA	162.8	144.8	142.2	129.2	90.5	9.6
M5PFPeA	158.2	144.1	140.1	136.8	90.5	6.5
M6PFDA	148.1	137.5	138.5	138.1	87.9	3.6
M7PFUnA	151.2	145.2	143.9	143.2	91.2	2.5
M8FOSA	155.3	149.2	131.9	135.2	89.3	7.8
M8PFOA	156.7	138.5	146.7	136.6	90.4	6.3
M8PFOS	141.2	139.1	136.7	120.8	84.1	6.9
M9PFNA	157.2	136.0	144.3	132.3	89.1	7.7

Table 9: Wastewater- Surrogates Recoveries: Accuracy (%recovery) and precision (%RSD) at 160 ng/L.

Sample ID	160 ng/L #1	160 ng/L #2	160 ng/L #3	160 ng/L #4	%Average Recovery (ng/L)	%RSD
d3-NMeFOSAA	158.1	145.7	150.1	138.8	92.6	5.4
d5-NEtFOSAA	161.7	153.8	147.5	141.7	94.5	5.7
M2-4-2 FTS	170.6	147.6	161.9	159.5	100.0	5.9
M2-6-2 FTS	146.9	157.1	146.2	143.0	92.7	4.1
M2-8-2 FTS	151.2	151.7	166.9	146.3	96.3	5.8
M2PFDoA	160.1	160.5	168.6	143.3	98.9	6.7
M2PFTreA	153.4	150.3	157.4	136.7	93.4	6.0
M3PFBS	179.4	165.4	163.8	151.9	103.2	6.8
M3PFHxS	169.9	151.6	160.2	144.6	97.9	7.0
M4PFBA	173.8	172.4	155.5	149.5	101.8	7.5
M4PFHpA	169.1	164.5	156.1	148.4	99.7	5.7
M5PFHxA	174.3	171.4	164.2	148.5	102.9	7.0
M5PFPeA	174.6	168.7	158.5	149.5	101.8	6.8
M6PFDA	154.4	154.1	155.1	134.8	93.5	6.6
M7PFUnA	156.5	156.9	167.9	139.5	97.0	7.6
M8FOSA	156.2	169.7	159.3	146.6	98.8	6.0
M8PFOA	166.2	156.4	162.5	150.2	99.3	4.4
M8PFOS	147.4	146.3	150.7	136.2	90.7	4.3
M9PFNA	159.8	157.6	164.5	142.3	97.6	6.2

■ Summary and Conclusions

The app note evaluated EPA SW-846 method 8327 for the direct injection analysis of 24 PFASs and 19 mass-labeled surrogates in non-potable waters (namely ground water, surface water and wastewater) using Shimadzu UFMSTM LCMS-8050. The data referenced in this article shows excellent performance of the LCMS-8050 for PFAS analysis in challenging environmental matrices with minimal sample preparation.

Good linearity, accuracy, and precision for all PFAS compounds included in draft EPA Method 8327 were achieved. Hence, the Shimadzu LCMS-8050 could achieve rapid, reliable and highly-sensitive quantitative results in non-potable waters, allowing for high-throughput and fast turnaround times.

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