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Application News

No. LCMS-150

Liquid Chromatography Mass Spectrometry

ASTM D8421-22 Standard Test Method for Determination of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous Matrices by Co-solvation Followed by Analysis Using the Shimadzu LCMS-8060NX

User Benefits

- The LCMS-8060NX easily meets and exceeds method performance criteria of ASTM D8421 for 44 PFAS and 24 surrogates.
- Optimized chromatography and MS conditions for excellent peak shape for improved precision and accuracy.
- ASTM D8421 is a simple extraction procedure validated by ASTM for the analysis of PFAS in wastewater samples.

■ Introduction and Background

ASTM International published ASTM D8421[1] for the analysis of 44 per- and polyfluorinated alkyl substances and 24 labeled isotopes in non-potable water samples. This method extracts the substances in a 1+1 ratio of sample and methanol, filters and then measures the targeted compounds using external standard calibration liquid chromatography-tandem mass spectrometry (LC/MS/MS). The minimum reporting limit is 10 ng/L with an analytical range of 10 – 400 ng/L for most compounds. The method requires standard solutions be prepared by the laboratory from neat compounds.

To save a laboratory's time and effort from preparing stock standards individually, we optimized the method using commercially available native and labeled calibration standard mixes. Additionally, we optimized chromatography, achieving better peak shape for early-eluting compounds, such as PFBA and PFPrA.

This application news summarizes the performance of the Shimadzu LCMS-8060NX Liquid Chromatography Mass Spectrometer (LC/MS/MS) (Figure 1) for all analytes listed in ASTM D8421. Results meet or exceed the requirements outlined in the method.

The reporting range and the target analytes are listed in Table 1. The reporting limit (RL) for the test method is defined as an integer value that is equal to the concentration of the lowest calibration standard.

Figure 1: Shimadzu LCMS-8060NX

Table 1: Analyte List with D8421 Reporting Range

Analyte Name	Acronym	CAS Number	Range (ng/L)
Perfluorotetradecanoic acid	PFTreA	376-06-7	10-400
Perfluorotridecanoic acid	PFTriA	72629-94-8	10-400
Perfluorododecanoic acid	PFDoA	307-55-1	10-400
Perfluoroundecanoic acid	PFUnA	2058-94-8	10-400
Perfluorodecanoic acid	PFDA	335-76-2	10-400
Perfluorononanoic acid	PFNA	375-95-1	10-400
Perfluorooctanoic acid	PFOA	335-67-1	10-400
Perfluoroheptanoic acid	PFHpA	375-85-9	10-400
Perfluorohexanoic acid	PFHxA	307-24-4	10-400
Perfluoropentanoic acid	PFPeA	2706-90-3	50-1000
Perfluorobutanoic acid	PFBA	375-22-4	50-1000
Perfluorodecanesulfonic acid	PFDS	335-77-3	10-400

Perfluorononanes`ulfonic acid	PFNS	68259-12-1	10-400
Perfluorooctanesulfonic acid	PFOS	1763-23-1	10-400
Perfluoroheptanesulfonic acid	PFHpS	375-92-8	10-400
Perfluorohexanesulfonic acid	PFHxS	355-46-4	10-400
Perfluoropentanesulfonic acid	PFPeS	2706-91-4	10-400
Perfluorobutanesulfonic acid	PFBS	375-73-5	10-400
Perfluorooctanesulfonamide	PFOSA	754-91-6	10-400
8:2 Fluorotelomer sulfonic acid	8:2 FTS	39108-34-4	10-400
6:2 Fluorotelomer sulfonic acid	6:2 FTS	27619-97-2	10-400
4:2 Fluorotelomer sulfonic acid	4:2 FTS	757124-72-4	10-400
N-Ethylperfluorooctanesulfonamidoacetic acid	NEtFOSAA	2991-50-6	10-400
N-Methylperfluorooctanesulfonamidoacetic acid	NMeFOSAA	2355-31-9	10-400
Perfluorododecanesulfonic acid	PFDoS	79780-39-5	10-400
N-Methylperfluorooctanesulfonamide	NMeFOSA	31506-32-8	10-400
N-Ethylperfluorooctanesulfonamide	NEtFOSA	4151-50-2	10-400
N-Methylperfluorooctanesulfonamidoethanol	NMeFOSE	24448-09-7	10-400
N-Ethylperfluorooctanesulfonamidoethanol	NEtFOSE	1691-99-2	10-400
Hexafluoropropylene oxide dimer acid	HFPO-DA	13252-13-6	10-400
4,8-dioxa-3H-perfluorononanoic acid	ADONA	919005-14-4	10-400
9-chlorohexadecafluoro-3-oxanonane-1-sulfonic acid	9Cl-PF3ONS	756426-58-1	10-400
11-chloroeicosafluoro-3-oxaundecane-1-sulfonic acid	11Cl-PF3OUdS	763051-92-9	10-400
Pentafluorpropanoic acid	PFPrA	422-64-0	50-1000
Perfluoro-3,6-dioxaheptanoic acid	NFDHA	151772-58-6	10-400
Perfluoro(2-ethoxyethane) sulfonic acid	PFEESA	113507-82-7	10-400
Perfluoro-3-methoxypropanoic acid	PFMPA	377-73-1	10-400
Perfluoro-4-methoxybutanoic acid	PFMBA	863090-89-5	10-400
2H,2H,3H,3H-Perfluorohexanoic Acid	3:3 FTCA	356-02-05	10-400
2H,2H,3H,3H-Perfluorooctanoic Acid	5:3 FTCA	914637-49-3	10-400
2H,2H,3H,3H-Perfluorodecanoic acid	7:3 FTCA	812-70-4	10-400
2H-perfluoro-2-octenoic acid	FHUEA	70887-88-6	10-400
2H-perfluoro-2-decenoic acid	FOUEA	70887-84-2	10-400
Lithium Bis(trifluoromethane)sulfonimide *	HQ-115	90076-65-6	10-400
Surrogates			
Perfluoro-n-[^{13}C4] butanoic acid	MPFBA	NA	10-400
Perfluor0-n-[$^{13}C_5$] pentanoic acid	M5PFPeA	NA	10-400
Perfluoro-n-[1,2,3,4,6-$^{13}C_5$] hexanoic acid	M5PFHxA	NA	10-400
Perfluoro-n-[1,2,3,4-$^{13}C_4$] heptanoic acid	M4PFHpA	NA	10-400
Perfluoro-n-[$^{13}C_8$] octanoic acid	M8PFOA	NA	10-400
Perfluoro-n-[$^{13}C_9$] nonanoic acid	M9PFNA	NA	10-400
Perfluoro-n-[1,2,3,4,5,6-$^{13}C_6$] decanoic acid	M6PFDA	NA	10-400
Perfluoro-n-[1,2,3,4,5,6,7-$^{13}C_7$] undecanoic acid	M7PFUnA	NA	10-400
Perfluoro-n-[1,2-$^{13}C_2$] dodecanoic acid	MPFDoA	NA	10-400
Perfluoro-n-[1,2-$^{13}C_2$] tetradecanoic acid	M2PFTreA	NA	10-400
Perfluoro-1-[$^{13}C_8$] octanesulfonamide	M8FOSA	NA	10-400
N-methyl-d_3-perfluoro-1-octanesulfonamidoacetic acid	D3-N-MeFOSAA	NA	10-400
N-ethyl-d_5-perfluoro-1-octanesulfonamidoacetic acid	D5-N-EtFOSAA	NA	10-400
N-methyl-d_3-perfluoro-1-octanesulfanamide	d-N-MeFOSA	NA	10-400
N-ethyl-d_5-perfluoro-1-octanesulfanamide	d-N-EtFOSA	NA	10-400
2-(N-methyl-d_3-perfluoro-1-octanesulfonamido) ethan-d_4-ol	d7-N-MeFOSE	NA	10-400
2-(N-ethyl-d_5-perfluoro-1-octanesulfonamido) ethan-d_4-ol	D9-N-EtFOSE	NA	10-400
2,3,3,3-Tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy-$^{13}C_3$-propanoic acid	MHFPO-DA	NA	10-400
1H,1H,2H,2H-perfluoro-1-[1,2-$^{13}C_2$] hexane sulfonate	M4:2FTS	NA	10-400
1H,1H,2H,2H-perfluoro-1-[1,2-$^{13}C_2$]-octane sulfonate	M6:2FTS	NA	10-400
1H,1H,2H,2H-perfluoro-1-[1,2-$^{13}C_2$]-decane sulfonate	M8:2FTS	NA	10-400
Perfluoro-1-[$^{13}C_8$] octanesulfonate	M8PFOS	NA	10-400
Perfluoro-1-[2,3,4-$^{13}C_3$] butanesulfonate	MPFBS	NA	10-400
Perfluoro-1-[1,2,3-$^{13}C_3$] hexanesulfonate	M3PFHxS	NA	10-400

Compounds in red are not in the Method 1633 standards and need to be added separately

■ Materials and Methods

Stock standard solutions containing native analytes and labeled isotopes (surrogates) were diluted from commercially available mixed stock standards (Wellington Method 1633 standard mixes) to be within the calibration range per analyte as shown in Table 1.

The individual standard solution was prepared in 50:50 (vol: vol) methanol/water with 0.1% acetic acid to obtain final concentrations shown in Table 2.

Table 2: Concentrations of each Calibration Standard (CS) in ng/L

	Compounds	CS1	CS2	CS3	CS4	CS5	CS6	CS7	CS8	CS9	CS10	CS11	CS12	CS13	CS14	CS15
Analyte	All analytes unless otherwise noted	1	2.5	5	10	25	40	60	80	100	150	200	250	375	500	800
	PFPeA	2	5	10	20	50	80	120	160	200	300	400	500	750	1000	1600
	PFBA, 4:2-FTS, 6:2-FTS, 8:2-FTS	4	10	20	40	100	160	240	320	400	600	800	1000	1500	2000	3200
	PFPrA, 5:3 FTCA, 7:3 FTCA	5	12.5	25	50	125	200	300	400	500	750	1000	1250	1875	2500	4000
	NMeFOSE, NEtFOSE	10	25	50	100	250	400	600	800	1000	1500	2000	2500	3750	5000	8000
Surrogate	13C9-PFNA, 13C6-PFDA, 13C7-PFUnA, 13C2-PFDoA, 13C2-PFTreA	0.25	0.625	1.25	2.5	6.25	10	15	20	25	37.5	50	62.5	93.75	125	200
	13C5-PFHxA, 13C4-PFHpA, 13C8-PFOA, 13C8-PFOSA, D3-NMeFOSA, D5-NEtFOSA, 13C8-PFOS, 13C3-PFBS, 13C3-PFHxS	0.5	1.25	2.5	5	12.5	20	30	40	50	75	100	125	187.5	250	400
	13C5-PFPeA, 13C2-4:2FTS, 13C2-6:2FTS, 13C2-8:2FTS, D3-NMeFOSAA, D5-NEtFOSAA	1	2.5	5	10	25	40	60	80	100	150	200	250	375	500	800
	13C4-PFBA, 13C3-HFPO-DA	2	5	10	20	50	80	120	160	200	300	400	500	750	1000	1600
	D7-NMeFOSE, D9-NEtFOSE	5	12.5	25	50	125	200	300	400	500	750	1000	1250	1875	2500	4000

These standards were not filtered. Calibration is performed using a 6 to 10-point curve, depending on the analyte. To obtain the calibration levels from the commercial stock solutions, 15 individual calibration standards were prepared and analyzed. Only the calibration points within the method-specified range were used.

The stock solutions were prepared and stored in PFAS-free polypropylene (PP) containers. Prior to the analysis, the solutions were shaken thoroughly, then transferred to a 2 mL PP LC vial and analyzed within 24 hours. If samples or standards are allowed to sit in the LC vials, some PFAS compounds may settle, rise, precipitate, or adsorb on the surface. To ensure a homogenous solution and optimum results, the solutions were vortexed prior to injection.

2.1 Sample Preparation

The surrogate spiking mix is added to 5 mL of sample contained in a 15 mL polypropylene vial. Add 5 mL of methanol and mix by vortex for ~2 minutes. After mixing, add acetic acid and adjust the pH ~4. Transfer an aliquot to a LC vial and cap with a Shimadzu GLC PP vial with septum confirmed to not contain PFAS. Analyze per the conditions shown in Table 3. Concentrations obtained from the curve are multiplied by two to obtain the final concentration in the samples.

2.2 Analytical Conditions

Table 3: Instrument Configuration and Analytical Conditions for ASTM D8421 PFAS using the Shimadzu LCMS-8060NX.

Mobile Phase	A: 2 mmol/L Ammonium Acetate in H_2O/ Acetonitrile = 95/5
	B: Acetonitrile
Delay Column	Shim-pack Scepter C18-120
	2.1 mm x 100 mm, 3 µm (P/N: 227-31014-05)
Analytical Column	Shim-pack GIST-HP C18
	3.0 mm x 100 mm, 3 um (P/N: 227-30040-04)
Gradient (%B)	10% (0 min) ⇒22% (2.3-3.0 min) ⇒ 45% (6.0 min) ⇒ 80% (13.0 min) ⇒ 95% (14.0-16 min) ⇒10% (16.01-20.0 min)
Interface	IonFocus ESI
Column Oven Temp.	40 °C
Flow rate	0.6 mL/min
Injection volume	25 µL
Multiple draw injection program	Co-injection 25 µL Sample → 25 µL 0.1% Acetic acid in H2O
Interface Temp.	170 ℃
Probe position	+3 mm
Neblizer gas flow	3 L/min
Heating gas flow	15 L/min
Interface Voltage	-0.5 kV (same value for all compounds)
DL Temp.	200 ℃
Heatblock Temp.	300 ℃
Drying gas flow	5 L/min
Focus bias	-2 kV (same value for all compounds)

■ Results and Discussion

A single laboratory validation of this method for specificity, linearity, recovery, and precision in nine wastewater matrices according to ASTM D8272[2] was previously described.[3] For this application news, a study was made to improve peak shape, particularly of early-eluting compounds, such as PFPrA and PFBA. This included evaluation of injection technique, columns, and flow rate. Co-injection of 25 µL sample with 25 µL 0.1% acetic acid in reagent water significantly improved the peak shapes of PFPrA, PFBA, and PFMPA (Figure 2). A large diameter column with a long column length and large particle size, combined with a high flow rate, allowed greater axial diffusion, improving peak shape (Figure 3).

Finally, to better separate impurities from the mobile phase, a new delay column was chosen, and the gradient program was modified (Figure 4). Upon optimization of chromatography and mass spectrometer conditions, calibration mixtures (Table 2) were prepared and used for subsequent analysis. Compound parameters, including quantitation ion, confirmation ion and collision energies, were optimized using LabSolutions software. At least two MRM transitions, if available, were used.

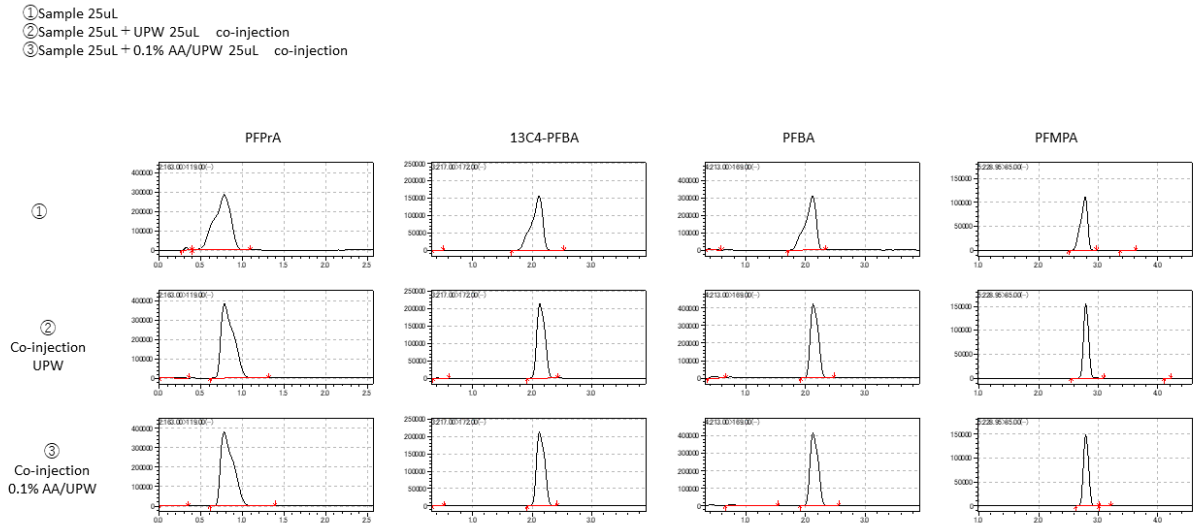

Figure 2: Optimization of injection technique to improve peak shape

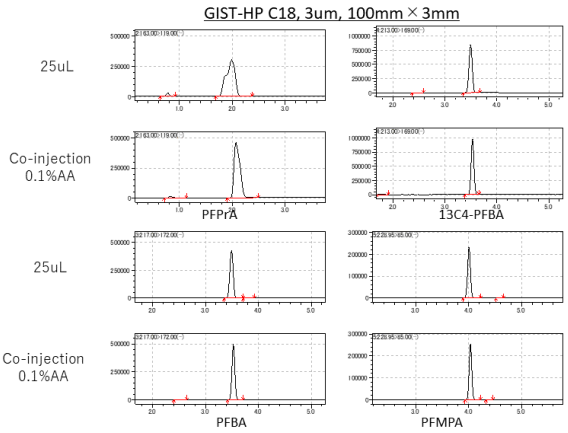

Figure 3: Example chromatograms for final column and flow rate with co-injection applied

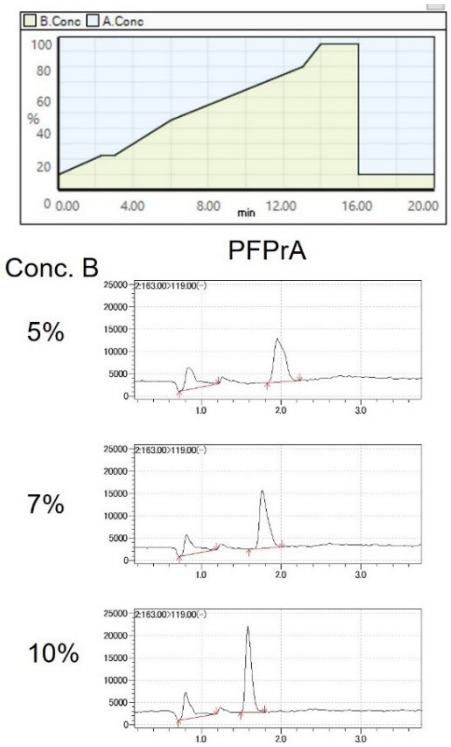

Figure 4: Final gradient with chromatogram of PFPrA, the earliest eluting peak

Linearity Study

Calibration curves for each analyte were found by Shimadzu Lab Solutions Insight data processing software to have a % RSD of less than 30%, as required by ASTM D8421. Calibration data, MRM transitions for the quantitation and confirmation ions (when available), and retention times are shown in Table 4. Calibration curves along with a midpoint standard chromatogram of PFOA and PFOS are shown in Figures 5 and 6.

These compounds were chosen to illustrate because of their likelihood for regulation in wastewater. Additionally, calibration curves and midpoint chromatograms of PFPrA and NEtFOSE are shown in Figures 7 and 8. These compounds were chosen because they are the earliest and latest eluting compounds respectively.

Table 4: Summary of calibration data.

Compound	Quantitation Ion	Confirmation Ion	Retention Time (min)	r^2
PFTreA	712.95>668.95	712.95>169.00	11.756	0.9962
PFTriA	662.95>618.95	662.95>169.00	11.026	0.9978
PFDoA	612.95>568.95	612.95>319.00	10.286	0.9987
PFUnA	562.95>518.95	562.95>269.00	9.543	0.9991
PFDA	512.95>468.95	512.95>219.00	8.813	0.9967
PFNA	462.95>418.95	462.95>219.00	8.11	0.9921
PFOA	412.95>369.00	412.95>169.00	7.451	0.9929
PFHpA	362.95>319.00	362.95>169.00	6.807	0.9989
PFHxA	312.95>269.00	312.95>119.00	6.028	0.9976
PFPeA	263.00>219.00	263.00>69.00	4.728	0.9996
PFBA	213.00>169.00	----	3.026	0.9985
PFDS	598.90>79.95	598.90>98.95	10.785	0.9971
PFNS	548.95>79.95	548.95>98.95	10.033	0.9975
PFOS	498.95>79.95	498.95>98.95	9.275	0.9951
PFHpS	448.95>79.95	448.95>98.95	8.522	0.9951
PFHxS	398.95>79.95	398.95>98.95	7.783	0.9917
PFPeS	348.95>79.95	348.95>98.95	7.059	0.9917
PFBS	298.95>79.95	298.95>98.95	6.17	0.9990
PFOSA	497.95>77.95	497.95>477.95	11.075	0.9979
8:2FTS	526.95>506.95	526.95>80.90	8.426	0.9976
6:2FTS	426.95>406.95	426.95>80.90	7.148	0.9960
4:2FTS	326.95>306.95	326.95>80.90	5.678	0.9970

NEtFOSAA	584.00>418.95	584.00>526.00	9.01	0.9950
NMeFOSAA	569.95>418.95	569.95>482.95	8.703	0.9929
PFDoS	698.90>79.95	698.90>98.95	12.228	0.9959
NMeFOSA	511.95>219.00	511.95>169.00	13.556	0.9956
NEtFOSA	526.00>219.00	526.00>169.00	14.149	0.9988
NMeFOSE	616.00>59.00	----	13.246	0.9996
NEtFOSE	630.00>59.00	----	13.853	0.9998
HFPO-DA	285.00>169.00	285.00>185.00	6.365	0.9971
ADONA	376.95>251.00	376.95>85.00	7.064	0.9980
9Cl-PF3ONS	530.90>350.95	532.90>352.95	9.809	0.9994
11Cl-PF3OUdS	630.90>450.95	632.90>452.95	11.308	0.9994
PFPrA	163.00>119.00	----	1.589	0.9996
NFDHA	294.95>201.00	294.95>85.00	5.937	0.9953
PFEESA	314.95>135.00	314.95>82.95	6.628	0.9978
PFMPA	228.95>85.00	----	3.656	0.9981
PFMBA	278.95>85.00	----	5.279	0.9979
3:3 FTCA	241.00>177.00	241.00>117.00	3.804	0.9717
5:3 FTCA	341.00>237.00	341.00>217.00	6.375	0.9945
7:3 FTCA	441.00>317.00	441.00>337.00	7.752	0.9964
FHUEA	357.00>293.00	----	6.472	0.9962
FOUEA	456.95>393.00	----	7.704	0.9973
HQ-115	279.90>146.95	279.90>210.90	7.259	0.9988
13C4-PFBA_Surr	217.00>172.00	----	3.023	0.9982
13C5-PFPeA_Surr	268.00>223.00	----	4.726	0.9976
13C5-PFHxA_Surr	318.00>273.00	318.00>120.00	6.026	0.9972
13C4-PFHpA_Surr	367.00>322.00	----	6.806	0.9994
13C8-PFOA_Surr	421.00>376.00	----	7.45	0.9959
13C9-PFNA_Surr	472.00>427.00	----	8.108	0.9947
13C6-PFDA_Surr	519.00>474.00	----	8.81	0.9989
13C7-PFUnA_Surr	570.00>525.00	----	9.541	0.9979
13C2-PFDoA_Surr	614.95>569.95	----	10.285	0.9968
13C2-PFTreA_Surr	714.95>669.95	----	11.755	0.9952
13C8-PFOSA_Surr	505.95>77.95	----	11.077	0.9983
D3-NMeFOSAA_Surr	573.00>418.95	----	8.697	0.9933
D5-NEtFOSAA_Surr	589.00>418.95	----	9	0.9976
D3-NMeFOSA_Surr	515.00>219.00	515.00>168.90	13.548	0.9993
D5-NEtFOSA_Surr	531.00>219.00	531.00>168.90	14.131	0.9983
D7-NMeFOSE_Surr	623.05>59.00	----	13.206	0.9957
D9-NEtFOSE_Surr	639.10>59.00	----	13.807	0.9994
13C3-HFPO-DA_Surr	287.00>169.00	284.90>185.00	6.363	0.9921
13C2-4:2FTS_Surr	329.00>308.95	329.00>80.90	5.678	0.9943
13C2-6:2FTS_Surr	428.95>408.95	428.95>80.90	7.147	0.9903
13C2-8:2FTS_Surr	528.95>508.95	528.95>80.90	8.425	0.9956
13C8-PFOS_Surr	506.95>79.95	506.95>98.95	9.274	0.9966
13C3-PFBS_Surr	301.95>79.95	301.95>98.95	6.17	0.9953
13C3-PFHxS_Surr	401.95>79.95	401.95>98.95	7.782	0.9921

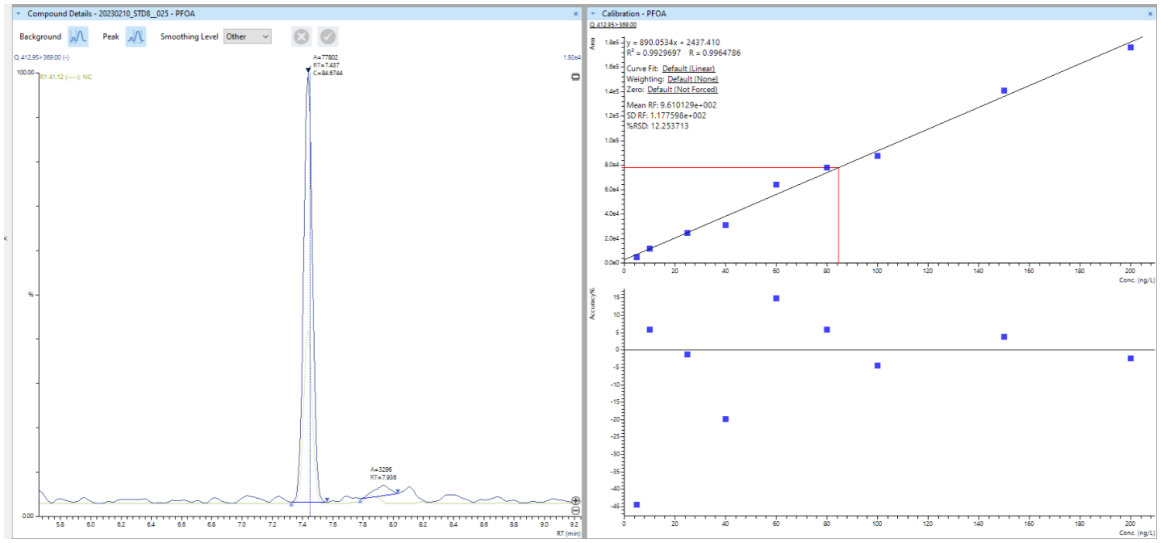

Figure 5: Calibration curve and midpoint chromatogram for PFOA

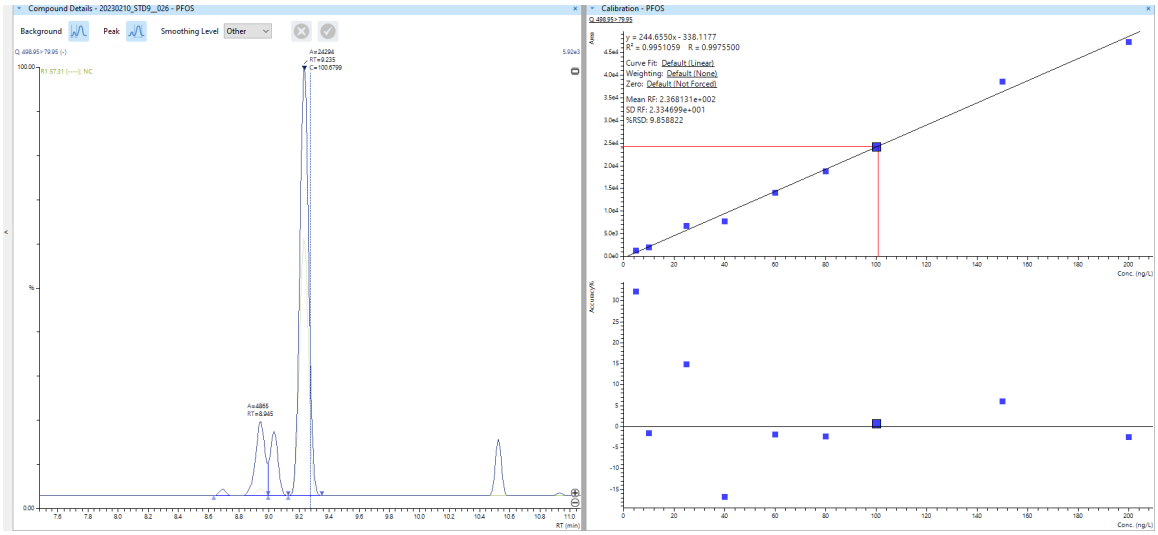

Figure 6: Calibration curve and midpoint chromatogram for PFOS

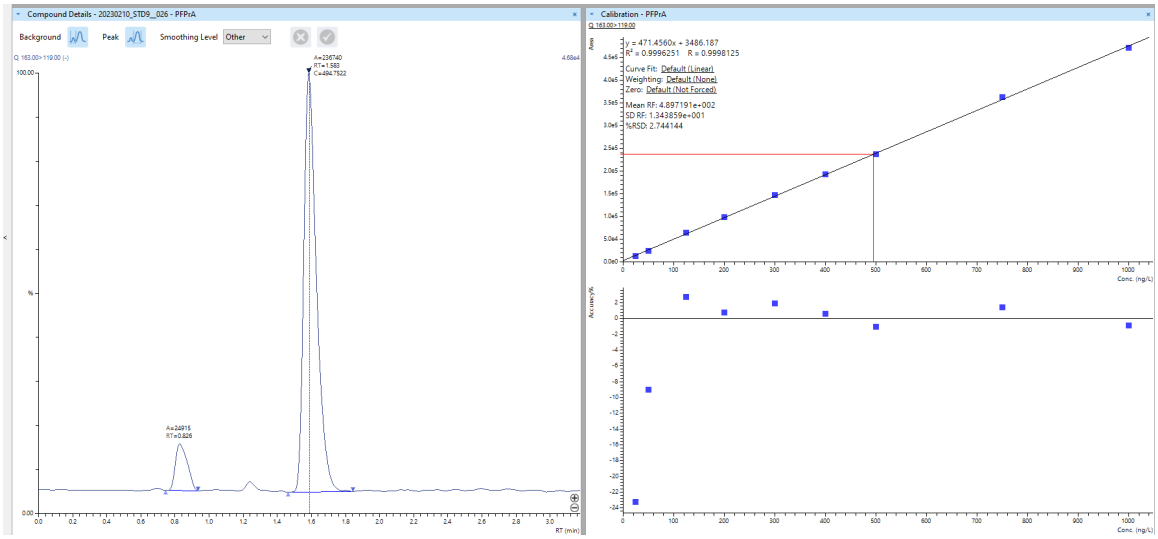

Figure 7: Calibration curve and midpoint chromatogram for PFPrA

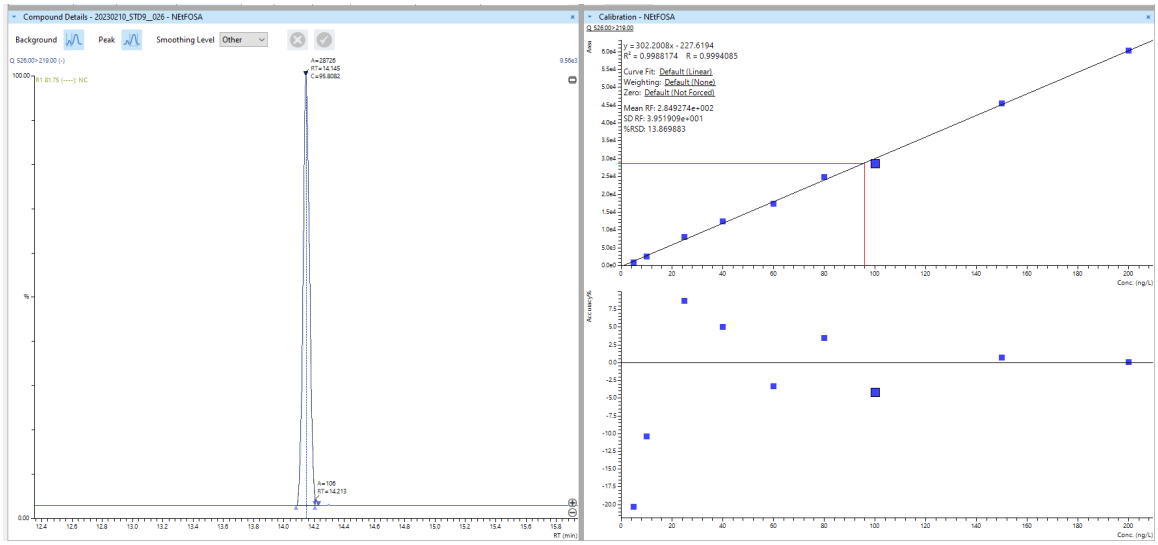

Figure 8: Calibration curve and midpoint chromatogram for NEtFOSE

Recovery and Repeatability Study

Recovery and repeatability (Table 5) were evaluated in reagent water and wastewater, each spiked four times at the concentration indicated. Recovery was calculated after subtracting the native PFAS found in the unspiked sample matrices.

These data are well within the 70 -130 % recovery and ≤ 30% RSD limits of the method.

Table 5: Recovery and Repeatability in Reagent Water and Wastewater

Compound	Spike Concentration (ppt)	Reagent Water % Recovery	Reagent Water %RSD (n=4)	Wastewater % Recovery	Wastewater %RSD (n=4)
PFTreA	160	110	3.76	119	2.71
PFTriA	160	109	2.08	79.9	4.82
PFDoA	160	104	4.33	107	4.6
PFUnA	160	113	5.53	105	2.49
PFDA	160	113	2.67	102	4.5
PFNA	160	113	6.71	107	2.34
PFOA	160	111	7.52	112	5.7
PFHpA	160	116	4.13	108	4.46
PFHxA	160	114	6.83	115	3.41
PFPeA	320	106	4.37	108	2.47
PFBA	640	107	0.55	108	2.06
PFDS	160	112	8.89	112	3.73
PFNS	160	113	3.72	116	5.58
PFOS	160	110	3.83	122	4.02
PFHpS	160	115	6.09	102	6.91
PFHxS	160	113	5.93	113	13.15
PFPeS	160	124	4.94	119	9.49
PFBS	160	109	4.59	114	5.12
PFOSA	160	101	2.44	100	4.59
8:2FTS	640	113	6.24	103	4.97
6:2FTS	640	119	3.2	107	3.3
4:2FTS	640	121	0.7	100	2.47
NEtFOSAA	160	113	7.5	89.4	10.15
NMeFOSAA	160	111	13.35	88.0	7.42
PFDoS	160	106	5.23	108	9.31
NMeFOSA	160	102	3.68	91.5	5.59
NEtFOSA	160	100	0.73	90.5	3.33
NMeFOSE	1600	97.2	0.34	93.6	0.94
NEtFOSE	1600	96.8	0.9	93.5	1.39
HFPO-DA	160	109	2.35	112	9.66
ADONA	160	110	1.01	104	4.22
9Cl-PF3ONS	160	111	2.01	111	1.92
11Cl-PF3OUdS	160	112	3.59	111	2.78
PFPrA	800	108	1.8	105	0.77
NFDHA	160	107	9.13	110	4.16
PFEESA	160	112	4.71	115	4.45
PFMPA	160	106	2.37	102	5.83
PFMBA	160	113	7.07	115	2.55
3:3 FTCA	160	87.1	20.57	94.8	14.52
5:3 FTCA	800	95.7	6.91	90.4	4.22
7:3 FTCA	800	92.5	2.56	88.8	2.73
FHUEA	160	99.1	3.91	95.3	2.16
FOUEA	160	102	4.2	97.2	3.5
HQ-115	160	112	2.56	111	0.78
Surrogates					
13C4-PFBA_Surr	320	102	1.7	96.4	2.88
13C5-PFPeA_Surr	160	108	6.03	96.4	3.36
13C5-PFHxA_Surr	80	110	3.7	101	5.35
13C4-PFHpA_Surr	80	104	6.43	105	5.99
13C8-PFOA_Surr	80	107	11.32	100	10.19
13C9-PFNA_Surr	40	98.2	13.76	92.2	17.29

13C6-PFDA_Surr	40	106	5.74	96.5	8.59
13C7-PFUnA_Surr	40	98.6	6.01	90.8	6.68
13C2-PFDoA_Surr	40	96.1	4.31	94.9	5.43
13C2-PFTreA_Surr	40	98.9	10.44	119	9.46
13C8-PFOSA_Surr	80	92.2	2.22	91.4	6.54
D3-NMeFOSAA_Surr	160	98.4	3.95	90.6	6.56
D5-NEtFOSAA_Surr	160	95.0	3.55	81.3	3.26
D3-NMeFOSA_Surr	80	89.3	12.1	82.6	8.57
D5-NEtFOSA_Surr	80	90.5	8.83	84.2	8.94
D7-NMeFOSE_Surr	800	88.8	0.49	85.4	1.68
D9-NEtFOSE_Surr	800	89.6	0.97	85.9	1.49
13C3-HFPO-DA_Surr	320	103	3.19	101	8.25
13C2-4:2FTS_Surr	160	116	3.15	96.2	6.88
13C2-6:2FTS_Surr	160	119	2.25	97.3	5.65
13C2-8:2FTS_Surr	160	104	0.73	97.4	7.53
13C8-PFOS_Surr	80	103	9.45	105	9.61
13C3-PFBS_Surr	80	121	5.06	94.0	6.33
13C3-PFHxS_Surr	80	116	9.99	108	6.65

■ Conclusion

This application news demonstrates the analysis of 44 PFAS and 24 surrogate compounds in non-potable water by ASTM D8421 using the Shimadzu LCMS-8060NX Liquid Chromatography Mass Spectrometer (LC/MS/MS). Chromatographic conditions were optimized to achieve excellent peak shape, even for the earliest eluting compounds, such as PFPrA and PFBA.

The highly sensitive Shimadzu LCMS-8060NX easily exceeds method performance criteria of the ASTM method and provides testing laboratories with highly accurate and reliable, repeatable results for PFAS in wastewater samples.

■ References

1. ASTM Test Method D8241 Determination of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous Matrices by Co-solvation followed by Liquid Chromatography Tandem Mass Spectrometry (LC/MS/MS)
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Shimadzu Corporation
www.shimadzu.com/an/

SHIMADZU SCIENTIFIC INSTRUMENTS, INC.
Applications Laboratory
7102 Riverwood Drive, Columbia, MD 21045
Phone: 800-477-1227 Fax: 410-381-1222
www.ssi.shimadzu.com

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