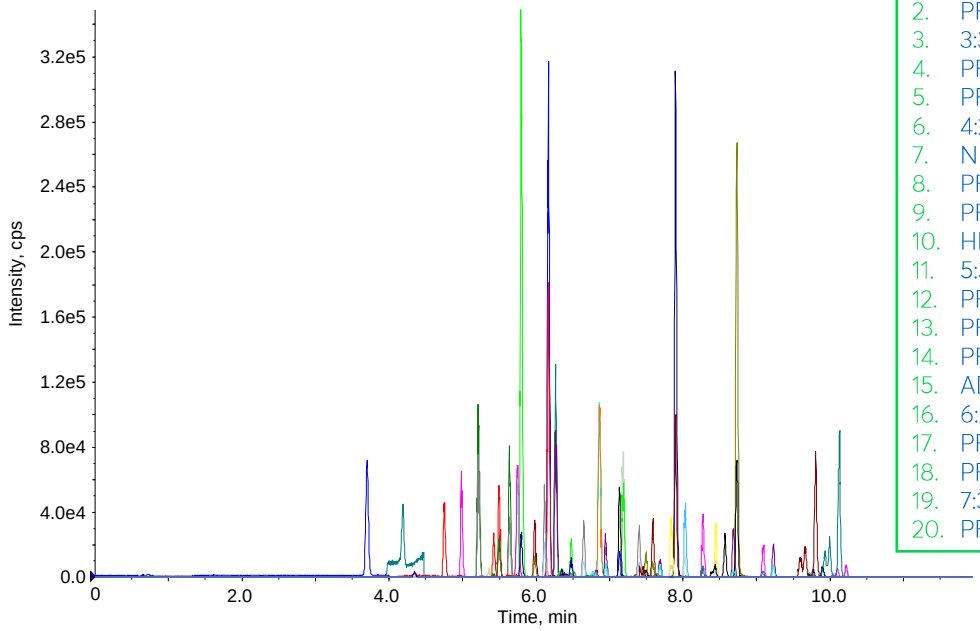
Chromatography Solutions

Application note #7860

LC-MS/MS analysis of 40 PFAS compounds specified in EPA method 1633



1.	PFBA	21.	PFHpS
2.	PFMPA	22.	8:2FTS
3.	3:3FTCA	23.	PFDA
4.	PFPeA	24.	NMeFOSAA
5.	PFMBA	25.	PFOS
6.	4:2FTS	26.	NEtFOSAA
7.	NFDHA	27.	PFUnA
8.	PFHxA	28.	9Cl-PF3ONS
9.	PFBS	29.	PFNS
10.	HFPO-DA	30.	PFDoA
11.	5:3FTCA	31.	PFDS
12.	PFEESA	32.	PFOSA
13.	PFHpA	33.	PFTrDA
14.	PFPeS	34.	11Cl-PF3OUdS
15.	ADONA	35.	PFTeDA
16.	6:2FTS	36.	PFDoS
17.	PFOA	37.	NMeFOSE
18.	PFHxS	38.	NMeFOSA
19.	7:3FTCA	39.	NEtFOSE
20.	PFNA	40.	NEtFOSA

Avantor® ACE®

Method Details

CONDITIONS

Column: Avantor® ACE® Excel® C18

Particle Size: 3 µm

Dimensions: 100 x 2.1 mm

Delay Column: Avantor® ACE® PFAS Delay Column

Dimensions: 50 x 2.1 mm

Mobile Phases: A: 5 mM ammonium acetate in H_2O (HiPerSolv CHROMANORM®, PFAS grade)

B: MeCN (HiPerSolv CHROMANORM®, PFAS grade)

Time (mins)	% B
0	5
0.5	5
10.5	95
11.5	95
11.6	5
14.6*	5

*The post column re-equilibration time may need to be adjusted for different LC systems

Flow Rate: 0.4 ml/min

Temperature: 40 °C

Injection volume: 4 µl

Detection: Sciex QTRAP® 6500+ LC-MS/MS system.

Ionisation mode: ESI, negative mode; Source temperature: 600 °C; Curtain gas: 30 psig; Ionspray™ source voltage: -4000 V; Source gas 1: 30 psig; Source gas 2: 50 psig

Sample: EPA1633 calibration standard with PFAS standards at 0.25 to 6.25 ng/l in MeOH:H_2O (96:4 v/v) +1% ammonium hydroxide +0.6% acetic acid.

MRM TRANSITIONS

Analyte	MRM	Optimised MS Parameters		
		Declustering potential (V)	Collision energy (V)	Cell exit potential (V)
1. PFBA (Perfluorobutanoic acid)	212.8 → 168.9	-5	-12	-15
2. PFMPA (Perfluoro-3-methoxypropanoic acid)	229.0 → 84.9	-5	-14	-11
3. 3:3FTCA (3-Perfluoropropyl propanoic acid)	241.0 → 177.0	-10	-10	-35
	241.0 → 117.0	-10	-44	-17
4. PFPeA (Perfluoropentanoic acid)	263.0 → 219.0	-5	-12	-11
	263.0 → 68.9	-5	-56	-9
5. PFMBA (Perfluoro-4-methoxybutanoic acid)	279.0 → 85.1	-5	-16	-9
6. 4:2FTS (*1H,1H, 2H, 2H*-Perfluorohexane sulfonic acid)	327.1 → 307.0	-30	-26	-17
	327.1 → 80.9	-50	-58	-9
7. NFDHA (Nonafluoro-3,6-dioxaheptanoic acid)	295.0 → 201.0	-5	-10	-9
	295.0 → 84.9	-10	-30	-9
8. PFHxA (Perfluorohexanoic acid)	313.0 → 269.0	-5	-12	-15
	313.0 → 118.9	-5	-26	-13
9. PFBS (Perfluorobutanesulfonic acid)	298.7 → 79.9	-70	-60	-9
	298.7 → 98.8	-75	-36	-11
10. HFPO-DA (Hexafluoropropylene oxide dimer acid)	284.9 → 168.9	-5	-10	-9
	284.9 → 184.9	-5	-24	-9
11. 5:3FTCA (*2H,2H,3H,3H*-Perfluorooctanoic acid)	341.0 → 237.1	-15	-18	-39
	341.0 → 217.0	-5	-34	-13
12. PFEESA (Perfluoro(2-ethoxyethane)sulfonic acid)	314.8 → 134.9	-55	-30	-27
	314.8 → 82.9	-50	-24	-39
13. PFHpA (Perfluoroheptanoic acid)	363.1 → 319.0	-5	-14	-17
	363.1 → 169.0	-5	-22	-9
14. PFPeS (Perfluoropentanesulfonic acid)	349.1 → 79.9	-85	-72	-9
	349.1 → 98.9	-50	-38	-11
15. ADONA (4,8-Dioxa-*3H*-perfluorononanoic acid)	376.9 → 250.9	-15	-16	-15
	376.9 → 84.8	-5	-34	-11
16. 6:2FTS (*1H,1H, 2H, 2H*-Perfluorooctane sulfonic acid)	427.1 → 407.0	-25	-32	-25
	427.1 → 80.9	-30	-70	-9

MRM TRANSITIONS

Analyte	MRM	Optimised MS Parameters		
		Declustering potential (V)	Collision energy (V)	Cell exit potential (V)
17. PFOA (Perfluorooctanoic acid)	413.0 → 369.0	-10	-14	-21
	413.0 → 169.0	-10	-24	-9
18. PFHxS (Perfluorohexanesulfonic acid)	398.7 → 79.9	-85	-76	-9
	398.7 → 98.9	-65	-78	-11
19. 7:3FTCA (3-Perfluoroheptyl propanoic acid)	441.0 → 316.9	-45	-32	-27
	441.0 → 336.9	-5	-16	-33
20. PFNA (Perfluorononanoic acid)	463.0 → 419.0	-5	-14	-25
	463.0 → 219.0	-10	-22	-11
21. PFHpS (Perfluoroheptanesulfonic acid)	449.0 → 79.9	-60	-86	-9
	449.0 → 98.9	-90	-88	-11
22. 8:2 FTS (*1H,1H, 2H, 2H*-Perfluorodecane sulfonic acid)	527.1 → 507.0	-20	-36	-33
	527.1 → 80.8	-5	-80	-9
23. PFDA (Perfluorodecanoic acid)	512.9 → 469.0	-5	-16	-23
	512.9 → 219.0	-10	-24	-11
24. NMeFOSAA (N-methyl perfluorooctanesulfonamidoacetic acid)	570.1 → 419.0	-15	-28	-29
	570.1 → 483.0	-20	-28	-29
25. PFOS (Perfluorooctanesulfonic acid)	498.9 → 79.9	-55	-90	-9
	498.9 → 98.9	-65	-94	-15
26. NEttFOSAA (N-ethyl perfluorooctanesulfonamidoacetic acid)	584.2 → 419.1	-15	-28	-25
	584.2 → 526.0	-15	-28	-25
27. PFUnA (Perfluoroundecanoic acid)	563.1 → 519.0	-5	-18	-29
	563.1 → 269.1	-15	-26	-15
28. 9Cl-PF3ONS (9-Chlorohexadecafluoro-3-oxanone-1-sulfonic acid)	530.8 → 351.0	-110	-34	-31
	530.8 → 353.0	-80	-36	-43
29. PFNS (Perfluorononanesulfonic acid)	548.8 → 79.9	-35	-98	-9
	548.8 → 98.9	-35	-98	-11
30. PFDoA (Perfluorododecanoic acid)	613.1 → 569.0	-15	-18	-35
	613.1 → 319.0	-25	-28	-17
31. PFDS (Perfluorodecanesulfonic acid)	599.0 → 79.9	-20	-98	-9
	599.0 → 98.9	-25	-106	-11

MRM TRANSITIONS

Analyte	MRM	Optimised MS Parameters		
		Declustering potential (V)	Collision energy (V)	Cell exit potential (V)
32. PFOSA (Perfluorooctanesulfonamide)	498.1 → 77.9	-45	-78	-9
	498.1 → 478.0	-25	-32	-23
33. PFTrDA (Perfluorotridecanoic acid)	663.0 → 619.0	-5	-18	-33
	663.0 → 168.9	-30	-36	-19
34. 11Cl-PF3OUdS (11-Chloroeicosafluoro-3-oxaundecane-1-sulfonic acid)	630.9 → 450.9	-45	-40	-29
	632.9 → 452.9	-50	-40	-43
35. PFTeDA (Perfluorotetradecanoic acid)	713.1 → 669.0	-25	-18	-39
	713.1 → 168.9	-25	-36	-21
36. PFDoS (Perfluorododecanesulfonic acid)	699.1 → 79.9	-30	-104	-9
	669.1 → 98.9	-45	-128	-13
37. NMeFOSE (N-methyl perfluorooctanesulfonamidoethanol)	616.1 → 58.9	-5	-52	-7
38. NMeFOSA (N-methyl perfluorooctanesulfonamide)	511.9 → 219.0	-30	-34	-11
	511.9 → 169.0	-50	-36	-19
39. NEtFOSE (N-ethyl perfluorooctanesulfonamidoethanol)	630.0 → 58.9	-40	-50	-17
40. NEtFOSA (N-ethyl perfluorooctanesulfonamide)	526.0 → 219.0	-10	-34	-11
	526.0 → 169.0	-15	-36	-19

ORDERING TABLE

Product	Details	Size	Part Number
Avantor® ACE® Excel® C18	HPLC Column	100 x 2.1 mm	EXL-111-1002U
Avantor® ACE® PFAS Delay Column	Pre-column trap	50 x 2.1 mm	ACE-PFASD-0502
Ammonium acetate 5 mM in water	VWR® HiPerSolv CHROMANORM® PFAS grade eluent for LC-MS	1 L	92500.290
Acetonitrile ≥99.9%	VWR® HiPerSolv CHROMANORM® PFAS grade for LC-MS	2.5 L	92497.320

RELATED PRODUCTS

Product	Details	Size	Part Number
Methanol ≥99.9%	VWR® HiPerSolv CHROMANORM® PFAS grade for LC-MS	2.5 L	92498.320
Water ≥99.9%	VWR® HiPerSolv CHROMANORM® PFAS grade for LC-MS	2.5 L	92499.320