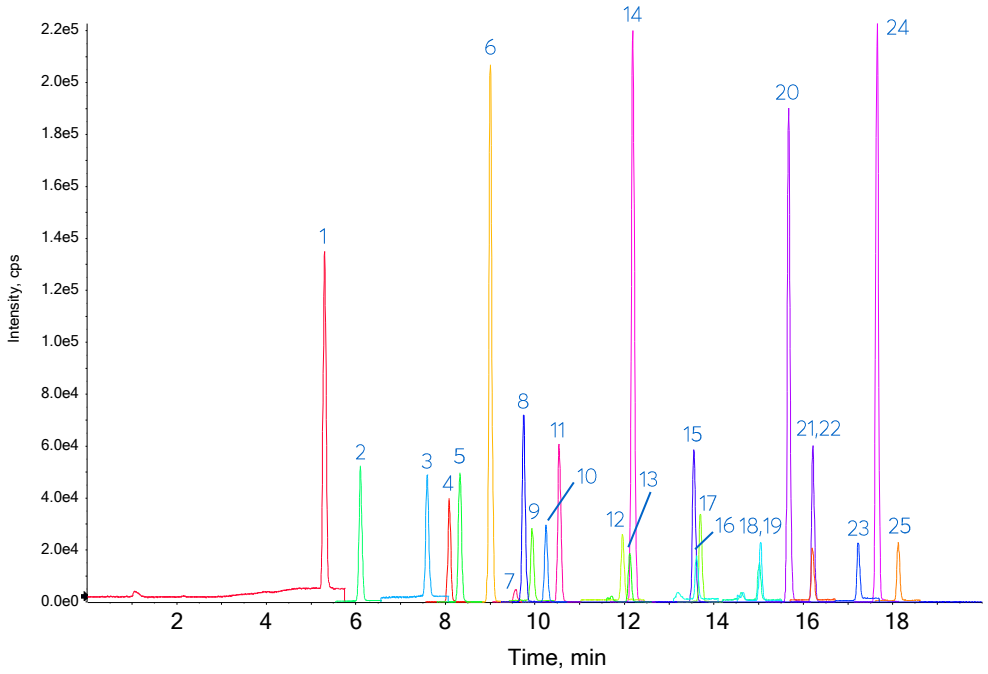
Chromatography Solutions

Application note #7840

Rapid LC-MS/MS analysis of PFAS compounds using EPA method 533



1. PFBA
2. PFMPA
3. PFPeA
4. PFBS
5. PFMBA
6. PFEESA
7. NFDHA
8. 4:2FTS
9. PFHxA
10. PFPeS
11. HFPO-DA
12. PFHpA
13. PFHxS
14. ADONA
15. 6:2FTS
16. PFOA
17. PFHpS
18. PFNA
19. PFOS
20. 9Cl-PF3ONS
21. 8:2FTS
22. PFDA
23. PFUnA
24. 11Cl-PF3OUdS
25. PFDoA

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: MeOH (HiPerSolv CHROMANORM®, PFAS grade)

Time (mins)	% B
0	5
0.5	5
3.0	40
16.0	80
18.0	80
20.0	95
22.0	95
25.0	5
35.0*	5

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

Flow Rate: 0.25 ml/min

Temperature: 40 °C

Injection volume: 5 µl

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

Ionisation mode: ESI, negative mode; Source temperature: 550 °C; Curtain gas: 35 psig; Ionspray™ source voltage: -3500 V; Source gas 1: 50 psig; Source gas 2: 60 psig

Sample: Calibration standard with PFAS standards at 100 to 2500 ng/L (corresponding to an in-sample concentration of 0.4 to 10.0 ng/L, taking into account 250x sample pre-concentration during sample preparation specified in EPA method 533).

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. PFPeA (Perfluoropentanoic acid)	263.0 → 219.0	-5	-12	-11
4. PFBS (Perfluorobutanesulfonic acid)	298.7 → 79.9	-70	-60	-9
5. PFMBA (Perfluoro-4-methoxybutanoic acid)	279.0 → 85.1	-5	-16	-9
6. PFEESA (Perfluoro(2-ethoxyethane)sulfonic acid)	314.8 → 134.9	-55	-30	-27
7. NFHDA (Nonafluoro-3,6-dioxaheptanoic acid)	295.0 → 201.0	-5	-10	-9
8. 4:2FTS (*1H,1H, 2H, 2H*-Perfluorohexane sulfonic acid)	327.1 → 307.0	-30	-26	-17
9. PFHxA (Perfluorohexanoic acid)	313.0 → 269.0	-5	-12	-15
10. PFPeS (Perfluoropentanesulfonic acid)	349.1 → 79.9	-85	-72	-9
11. HFPO-DA (Hexafluoropropylene oxide dimer acid)	284.9 → 168.9	-5	-10	-9
12. PFHpA (Perfluoroheptanoic acid)	363.1 → 319.0	-5	-14	-17
13. PFHxS (Perfluorohexanesulfonic acid)	398.7 → 79.9	-85	-76	-9
14. ADONA (4,8-Dioxa-3H-perfluorononanoic acid)	376.9 → 250.9	-15	-16	-15
15. 6:2FTS (*1H,1H, 2H, 2H*-Perfluorooctane sulfonic acid)	427.1 → 407.0	-25	-32	-25
16. PFOA (Perfluorooctanoic acid)	413.0 → 369.0	-10	-14	-21
17. PFHpS (Perfluoroheptanesulfonic acid)	449.0 → 79.9	-60	-86	-9
18. PFNA (Perfluorononanoic acid)	463.0 → 419.0	-5	-14	-25
19. PFOS (Perfluorooctanesulfonic acid)	498.9 → 79.9	-55	-90	-9
20. 9Cl-PF3ONS (9-Chlorohexadecafluoro-3-oxanone-1-sulfonic acid)	530.8 → 351.0	-110	-34	-31
21. 8:2FTS (*1H,1H, 2H, 2H*-Perfluorodecane sulfonic acid)	527.1 → 507.0	-20	-36	-33
22. PFDA (Perfluorodecanoic acid)	512.9 → 469.0	-5	-16	-23
23. PFUnA (Perfluoroundecanoic acid)	563.1 → 519.0	-5	-18	-29
24. 11Cl-PF3OUdS (11-Chloroeicosafluoro-3-oxaundecane-1-sulfonic acid)	630.9 → 450.9	-45	-40	-29
25. PFDoA (Perfluorododecanoic acid)	613.1 → 569.0	-15	-18	-35

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
Methanol ≥99.9%	VWR® HiPerSolv CHROMANORM® PFAS grade for LC-MS	2.5 L	92498.320

RELATED PRODUCTS

Product	Details	Size	Part Number
Acetonitrile ≥99.9%	VWR® HiPerSolv CHROMANORM® PFAS grade for LC-MS	2.5 L	92497.320
Water ≥99.9%	VWR® HiPerSolv CHROMANORM® PFAS grade for LC-MS	2.5 L	92499.320