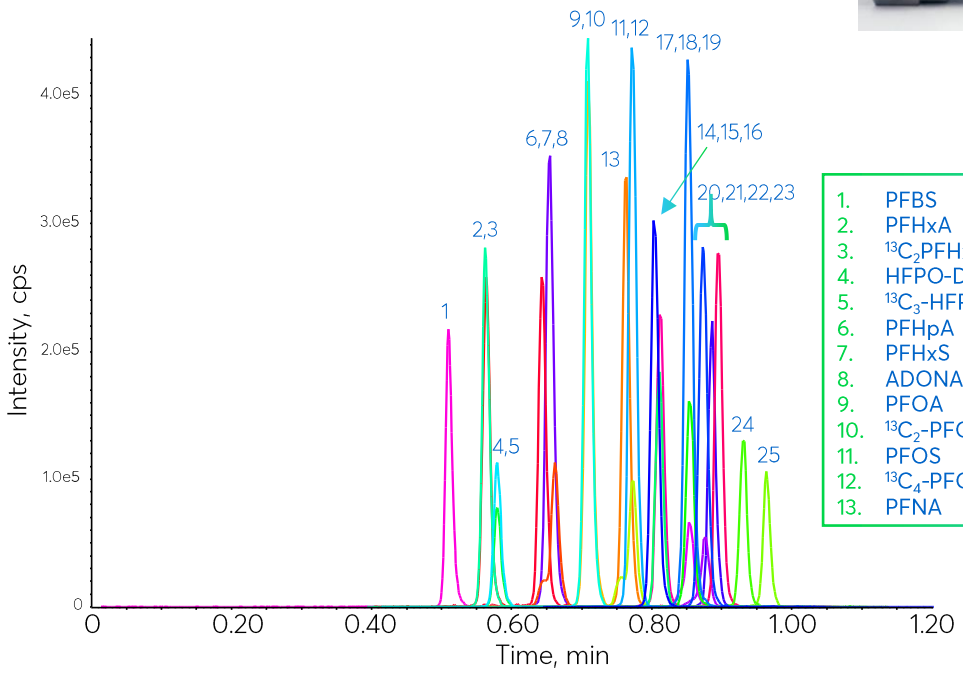
Chromatography Solutions

Application note #7830

Rapid LC-MS/MS screening of 18 PFAS compounds using an Avantor® ACE® HTP-MS column



1. PFBS
2. PFHxA
3. $^{13}C_2$PFHxA
4. HFPO-DA
5. $^{13}C_3$-HFPO-DA
6. PFHpA
7. PFHxS
8. ADONA
9. PFOA
10. $^{13}C_2$-PFOA
11. PFOS
12. $^{13}C_4$-PFOS
13. PFNA
14. 9Cl-PF3ONS
15. PFDA
16. $^{13}C_2$-PFDA
17. NMeFOSAA
18. d_3-NMeFOSAA
19. PFUnA
20. NEtFOSAA
21. d_5-NEtFOSAA
22. 11Cl-PF3OUdS
23. PFDoA
24. PFTrDA
25. PFTA

Avantor® ACE®

Method Details

CONDITIONS

Column: Avantor® ACE® HTP-MS

Particle Size: 2 µm

Dimensions: 10 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

B: MeOH

Time (mins)	% B
0	5
0.05	40
1.0	100
1.2	100
1.3	5
1.6	5

Flow Rate: 1.0 mL/min

Temperature: 22 °C

Injection volume: 4 µL

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

Ionisation mode: ESI, negative mode; Source temperature: 450 °C; Curtain gas: 38 psig; Ionspray™ source voltage: -4500 V; Ion source gas 1: 40 psig; Ion source gas 2: 70 psig.

Sample: Calibration standard with PFAS standards at 1000-4000 ng/L, internal standards and surrogate standards at 1000-4000 ng/L in MeOH:H_2O (1:1, v/v).

MRM TRANSITIONS

Analyte	MRM	Optimised MS Parameters		
		Declustering potential (V)	Collision energy (V)	Cell exit potential (V)
1. PFBS (Perfluorobutanesulfonic acid)	-298.8 → -79.9	-60	-66	-13
2. PFHxA (Perfluorohexanoic acid)	-312.8 → -268.8	-5	-12	-29
3. $^{13}C_2$PFHxA (Surrogate standard)	-314.8 → -269.9	-5	-12	-17
4. HFPO-DA (Hexafluoropropylene oxide dimer acid)	-285.0 → -169.0	-5	-10	-35
5. $^{13}C_3$-HFPO-DA (Surrogate standard)	-286.8 → -168.9	-10	-10	-15
6. PFHpA (Perfluoroheptanoic acid)	-362.8 → -318.8	-5	-14	-25
7. PFHxS (Perfluorohexanesulfonic acid)	-398.8 → -79.9	-5	-86	-9
8. ADONA (4,8-Dioxa-3H-perfluorononanoic acid)	-376.8 → -250.8	-15	-16	-23
9. PFOA (Perfluorooctanoic acid)	-412.8 → -368.9	-10	-14	-23
10. $^{13}C_2$-PFOA (Internal standard)	-414.8 → -369.8	-10	-14	-19
11. PFOS (Perfluorooctanesulfonic acid)	-498.8 → -79.9	-5	-102	-9
12. $^{13}C_4$-PFOS (Internal standard)	-502.8 → -79.9	-5	-104	-9
13. PFNA (Perfluorononanoic acid)	-462.8 → -418.8	-5	-16	-23
14. 9Cl-PF3ONS (9-Chlorohexadecafluoro-3-oxanone-1-sulfonic acid)	-530.7 → -350.8	-20	-36	-29
15. PFDA (Perfluorodecanoic acid)	-512.8 → -468.8	-25	-16	-45
16. $^{13}C_2$-PFDA (Surrogate standard)	-514.8 → -469.8	-5	-16	-25
17. NMeFOSAA (N-methyl perfluorooctanesulfonamidoacetic acid)	-569.8 → -418.8	-5	-30	-29
18. d_3-NMeFOSAA (Internal standard)	-572.8 → -418.9	-5	-30	-29
19. PFUnA (Perfluoroundecanoic acid)	-562.8 → -518.7	-5	-18	-33
20. NEtFOSAA (N-ethyl perfluorooctanesulfonamidoacetic acid)	-583.8 → -418.9	-30	-28	-19
21. d_5-NEtFOSAA (Surrogate standard)	-588.8 → -418.9	-25	-28	-21
22. 11Cl-PF3OUdS (11-Chloroeicosafluoro-3-oxaundecane-1-sulfonic acid)	-630.7 → -450.8	-5	-42	-23
23. PFDoA (Perfluorododecanoic acid)	-612.7 → -568.8	-10	-18	-35
24. PFTrDA (Perfluorotridecanoic acid)	-662.7 → -618.7	-15	-20	-35
25. PFTA (Perfluorotetradecanoic acid)	-712.7 → -668.6	-5	-20	-41

ORDERING TABLE

Product	Details	Size	Part Number
Avantor® ACE® HTP-MS Starter Kit	Fast Analysis LC-MS column (Holder & Cart)	10 x 2.1 mm	ACE-HTP-SK1
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
Water ≥99.9%	VWR® HiPerSolv CHROMANORM® PFAS grade for LC-MS	2.5 L	92499.320

RELATED PRODUCTS

Product	Details	Size	Part Number
Avantor® ACE® HTP-MS replacement cartridges, 3/pack	Replacement LC-MS column cartridge, 3/pack (requires holder)	10 x 2.1 mm	ACE-HTP3-0102
Avantor® ACE® HTP-MS replacement cartridges, 5/pack	Replacement LC-MS column cartridge, 5/pack (requires holder)	10 x 2.1 mm	ACE-HTP5-0102
Avantor® ACE® HTP-MS replacement cartridges, 10/pack	Replacement LC-MS column cartridge, 10/pack (requires holder)	10 x 2.1 mm	ACE-HTPX-0102
Avantor® ACE® HTP-MS replacement ferrules, 10/pack	Replacement ferrules for HTP-MS holder, 10/pack	-	F0001
Acetonitrile ≥99.9%	VWR® HiPerSolv CHROMANORM® PFAS grade for LC-MS	2.5 L	92497.320