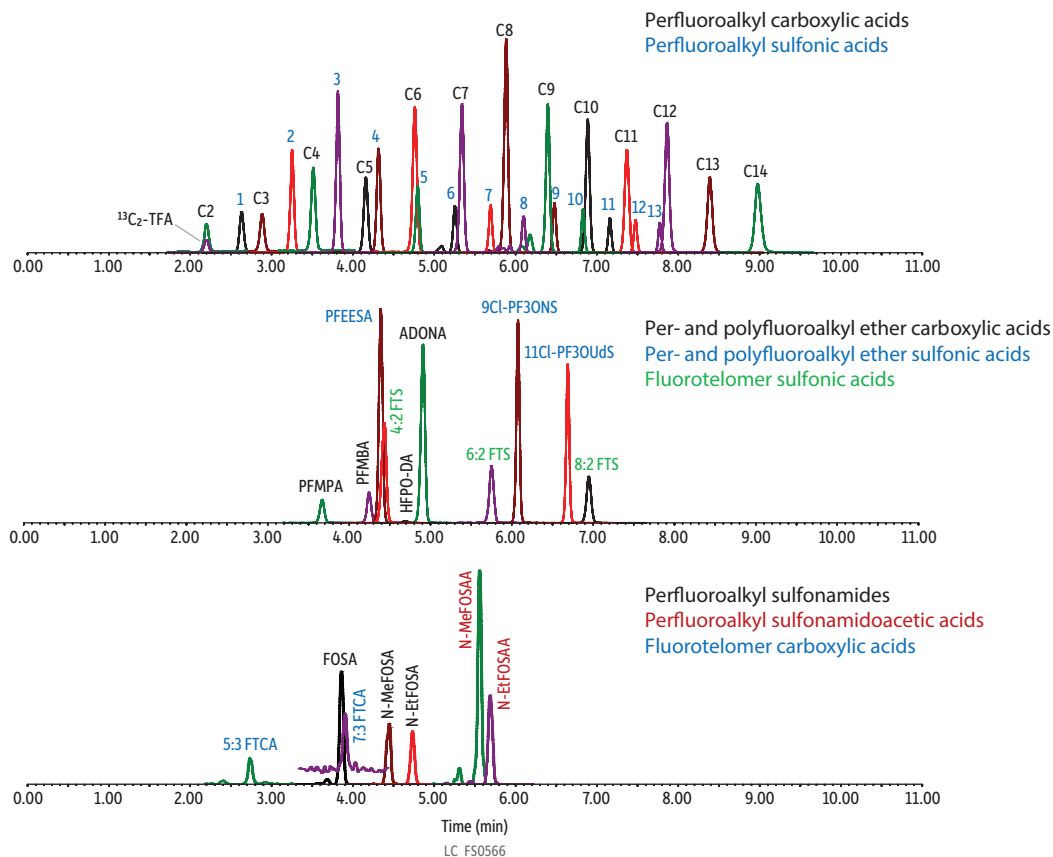


Integrating Ultrashort-Chain Compounds into Comprehensive PFAS Analysis in Beverage on Ultra IBD Inert



Column	Ultra IBD Inert (cat.# 9175312-T)		
Dimensions:	100 mm x 2.1 mm ID		
Particle Size:	3 µm		
Pore Size:	100 Å		
Temp.:	40 °C		
Standard/Sample	PFAS 28 calibration standard (cat.# 30734) Other standards were obtained externally.		
Diluent:	50:50 Water:acetonitrile		
Conc.:	The blend berry juice was fortified at 500 ng/L and diluted two-fold with acetonitrile.		
Inj. Vol.:	20 µL		
Mobile Phase			
A:	Water, 2mM ammonium formate, 0.1% formic acid		
B:	95:5 Acetonitrile:water, 2mM ammonium formate, 0.1% formic acid		
Time (min)	Flow (mL/min)	%A	%B
0.00	0.4	50	50
7.00	0.4	0	100
10.00	0.4	0	100
10.01	0.4	50	50
12.00	0.4	50	50
Max Pressure:	540 bar		
Detector	Waters Xevo TQ-S		
Ion Source:	Waters Zspray ESI		
Ion Mode:	ESI-		
Mode:	MRM		
Instrument	Waters ACQUITY UPLC I-Class		
Sample Preparation	The blend berry juice (0.5 mL) was transferred into a 15 mL polypropylene centrifuge tube, fortified at 500 ng/L, and mixed with 0.5 mL of acetonitrile by vortexing for 30 seconds. The mixture was then centrifuged at 4000 rpm, and the resulting supernatant was transferred to polypropylene HPLC vials for LC-MS/MS analysis.		
Notes	The confirmation ion peaks were not shown in the chromatogram. An Ultra IBD column (150 x 2.1 mm, 3.0 µm; cat # 9175362) was used as the delay column. For the chromatograms of perfluoroalkyl carboxylic and sulfonic acids, the peak numbers correspond to the carbon chain lengths of the PFAS compounds.		

Peaks	tr (min)	Conc. (ng/L)	Precursor Ion	Quantification Ion	Confirmation Ion
1. Trifluoroacetic acid (TFA)	2.20	250	113.03	69.01	-
2. 13C2-Trifluoroacetic acid (13C2-TFA)	2.20	250	114.90	69.95	-
3. Trifluoromethanesulfonic acid (TFMS)	2.63	250	148.97	79.93	98.92
4. 3-Perfluoropentyl propanoic acid (5:3 FTCA)	2.73	250	340.93	216.96	236.93
5. Perfluoropropanoic acid (PFPrA)	2.88	250	162.97	119.02	-
6. Perfluoroethanesulfonic acid (PFEtS)	3.25	250	198.90	79.92	98.91
7. Perfluorobutanoic acid (PFBA)	3.51	250	213.03	168.98	-
8. Perfluoro-3-methoxypropanoic acid (PFMPA)	3.68	250	228.93	84.97	198.94
9. Perfluoropropanesulfonic acid (PFPrS)	3.81	250	248.97	79.92	98.91
10. Perfluorooctanesulfonamide (FOSA)	3.87	250	498.17	77.97	477.76
11. 3-Perfluoroheptyl propanoic acid (7:3 FTCA)	3.92	250	440.90	336.88	316.91
12. Perfluoro(2-ethoxyethane)sulfonic acid (PFEESA)	4.09	250	314.83	134.94	83.01
13. Perfluoropentanoic acid (PFPeA)	4.16	250	262.97	218.97	-
14. Perfluoro-4-methoxybutanoic acid (PFMBA)	4.24	250	278.87	84.96	234.93
15. Perfluorobutanesulfonic acid (PFBS)	4.32	250	298.97	79.97	98.89
16. 1H,1H,2H,2H-Perfluorohexane sulfonic acid (4:2 FTS)	4.44	250	327.10	307.08	80.83
17. N-methyl perfluorooctanesulfonamide (NMeFOSA)	4.45	250	511.77	168.95	218.91
18. Hexafluoropropylene oxide dimer acid (HFPO-DA)	4.68	250	285.03	169.02	185.02
19. N-ethyl perfluorooctanesulfonamide (NEtFOSA)	4.73	250	525.83	168.96	218.92
20. Perfluorohexanoic acid (PFHxA)	4.76	250	313.10	268.97	118.99
21. Perfluoropentanesulfonic acid (PFPeS)	4.79	250	349.10	79.98	98.98
22. 4,8-Dioxo-3H-perfluorononanoic acid (ADONA)	4.90	250	376.90	250.93	84.97
23. Perfluorohexanesulfonic acid (PFHxS)	5.25	250	398.90	79.97	98.89
24. Perfluoroheptanoic acid (PFHpA)	5.34	250	363.16	319.09	169.06
25. N-methyl perfluorooctanesulfonamidoacetic acid (NMeFOSAA)	5.55	250	570.20	419.17	483.16
26. N-ethyl perfluorooctanesulfonamidoacetic acid (NEtFOSAA)	5.68	250	584.20	419.18	483.11
27. Perfluoroheptanesulfonic acid (PFHpS)	5.69	250	449.17	79.98	98.97
28. 1H,1H,2H,2H-Perfluorooctane sulfonic acid (6:2 FTS)	5.75	250	427.17	407.18	80.71
29. Perfluorooctanoic acid (PFOA)	5.88	250	413.10	368.96	168.90
30. 9-Chlorohexadecafluoro-3-oxanonane-1-sulfonic acid (9Cl-PF3ONS)	6.08	250	530.78	350.85	82.96
31. Perfluorooctanesulfonic acid (PFOS)	6.11	250	499.03	79.92	98.90
32. Perfluorononanoic acid (PFNA)	6.40	250	463.10	419.01	219.02
33. Perfluorononanesulfonic acid (PFNS)	6.48	250	549.10	79.92	98.83
34. 11-Chloroeicosafluoro-3-oxaundecane-1-sulfonic acid (11Cl-PF3OUdS)	6.69	250	630.78	450.80	82.95
35. Perfluorodecanesulfonic acid (PFDS)	6.83	250	599.17	79.98	98.83
36. Perfluorodecanoic acid (PFDA)	6.89	250	513.17	469.16	219.06
37. 1H,1H,2H,2H-Perfluorodecane sulfonic acid (8:2 FTS)	6.94	250	527.17	507.16	80.83
38. Perfluoroundecanesulfonic acid (PFUdS)	7.16	250	648.73	79.94	98.94
39. Perfluoroundecanoic acid (PFUnA)	7.37	250	563.23	519.24	269.07
40. Perfluorododecanesulfonic acid (PFDoS)	7.47	250	698.77	79.95	98.94
41. Perfluorotridecanesulfonic acid (PFTriDS)	7.77	250	748.73	79.94	98.94
42. Perfluorododecanoic acid (PFDoA)	7.86	250	613.23	569.19	169.06
43. Perfluorotridecanoic acid (PFTriDA)	8.38	250	663.23	619.21	169.06
44. Perfluorotetradecanoic acid (PFTeDA)	8.98	250	712.67	668.69	168.94