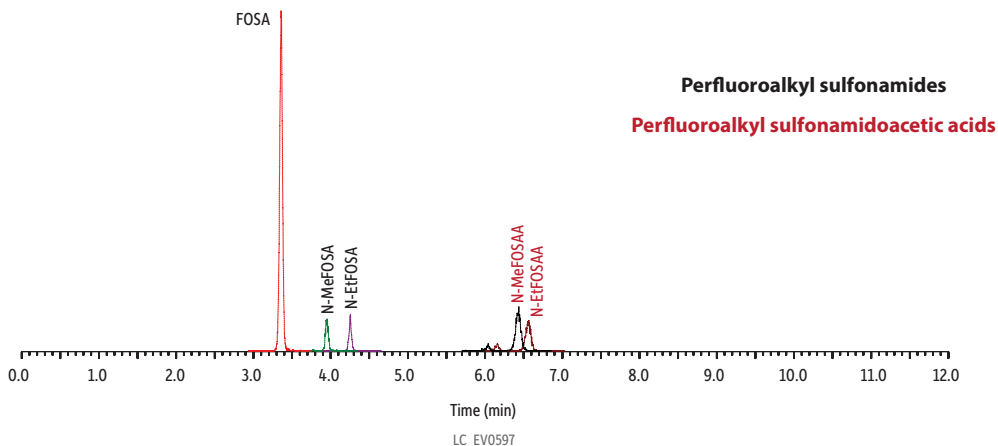
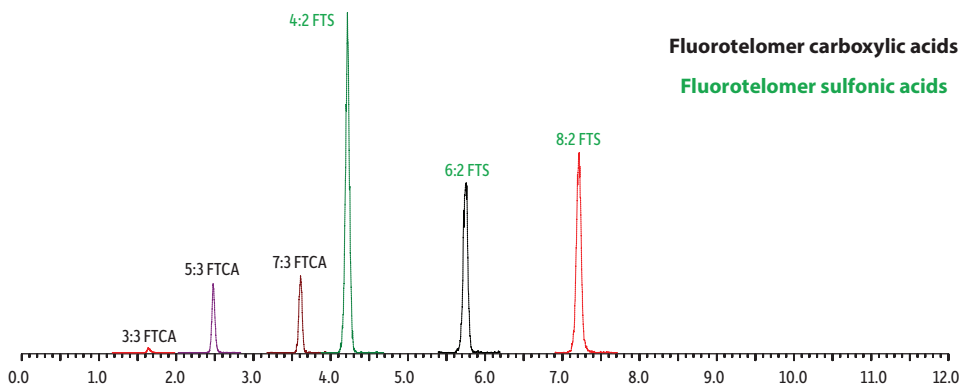
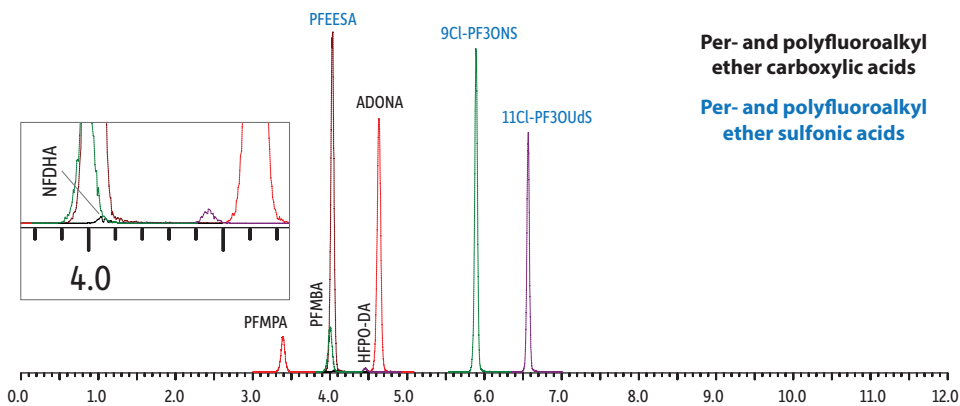
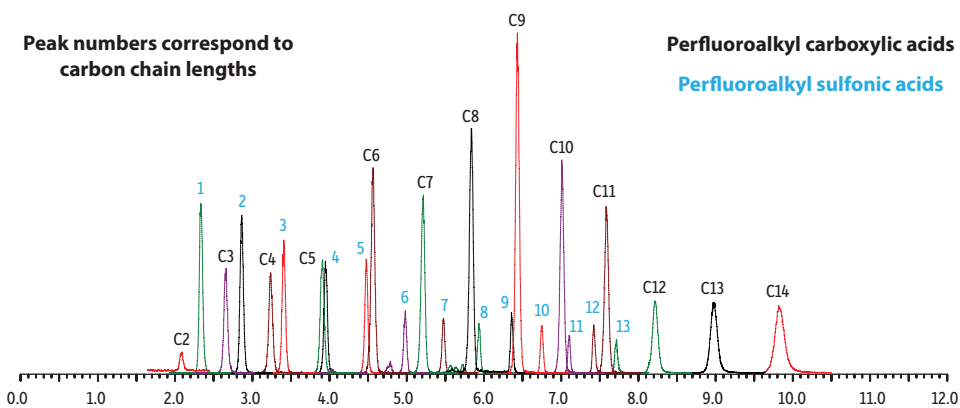


Incorporating Ultrashort-Chain Compounds into the Comprehensive Analysis of PFAS in Water Matrices on Ultra Inert IBD



| Peaks | tr (min) | Precursor Ion | Quantification Ion | Confirmation Ion |
|---------------------------------------------------------------------------------------------|----------|---------------|--------------------|------------------|
| 1. 3-Perfluoropropyl propanoic acid (3:3 FTCA) | 1.64 | 241.00 | 177.00 | 117.00 |
| 2. Trifluoroacetic acid (TFA) | 2.12 | 113.03 | 69.01 | - |
| 3. Trifluoromethanesulfonic acid (TFMS) | 2.36 | 148.97 | 79.93 | 98.92 |
| 4. 3-Perfluoropentyl propanoic acid (5:3 FTCA) | 2.49 | 340.93 | 216.96 | 236.93 |
| 5. Perfluoropropanoic acid (PFPrA) | 2.69 | 162.97 | 119.02 | - |
| 6. Perfluoroethanesulfonic acid (PFEtS) | 2.89 | 198.90 | 79.92 | 98.91 |
| 7. Perfluorobutanoic acid (PFBA) | 3.27 | 213.03 | 168.98 | - |
| 8. Perfluorooctanesulfonamide (FOSA) | 3.36 | 498.17 | 77.97 | 477.76 |
| 9. Perfluoro-3-methoxypropanoic acid (PFMPA) | 3.40 | 228.93 | 84.97 | 198.94 |
| 10. Perfluoropropanesulfonic acid (PFPrS) | 3.44 | 248.97 | 79.92 | 98.91 |
| 11. 3-Perfluoroheptyl propanoic acid (7:3 FTCA) | 3.61 | 440.90 | 336.88 | 316.91 |
| 12. Perfluoropentanoic acid (PFPeA) | 3.94 | 262.97 | 218.97 | - |
| 13. <i>N</i> -methyl perfluorooctanesulfonamide (NMeFOSA) | 3.96 | 511.77 | 168.95 | 218.91 |
| 14. Perfluorobutanesulfonic acid (PFBS) | 3.97 | 298.97 | 79.97 | 98.89 |
| 15. Perfluoro-4-methoxybutanoic acid (PFMBA) | 4.00 | 278.87 | 84.96 | 234.93 |
| 16. Perfluoro(2-ethoxyethane)sulfonic acid (PFEESA) | 4.04 | 314.83 | 134.94 | 83.01 |
| 17. Nonafluoro-3,6-dioxahexanoic acid (NFDHA) | 4.06 | 294.93 | 200.91 | 85.02 |
| 18. 1 <i>H</i> ,1 <i>H</i> ,2 <i>H</i> ,2 <i>H</i> -Perfluorohexane sulfonic acid (4:2 FTS) | 4.22 | 327.10 | 307.08 | 80.83 |
| 19. <i>N</i> -ethyl perfluorooctanesulfonamide (NEtFOSA) | 4.26 | 525.83 | 168.96 | 218.92 |
| 20. Hexafluoropropylene oxide dimer acid (HFPO-DA) | 4.46 | 285.03 | 169.02 | 185.02 |
| 21. Perfluoropentanesulfonic acid (PFPeS) | 4.50 | 349.10 | 79.98 | 98.98 |
| 22. Perfluorohexanoic acid (PFHxA) | 4.59 | 313.10 | 268.97 | 118.99 |
| 23. 4,8-Dioxa-3 <i>H</i> -perfluorononanoic acid (ADONA) | 4.63 | 376.90 | 250.93 | 84.97 |
| 24. Perfluorohexanesulfonic acid (PFHxS) | 5.01 | 398.90 | 79.97 | 98.89 |
| 25. Perfluoroheptanoic acid (PFHpA) | 5.24 | 363.16 | 319.09 | 169.06 |
| 26. Perfluoroheptanesulfonic acid (PFHpS) | 5.50 | 449.17 | 79.98 | 98.97 |
| 27. 1 <i>H</i> ,1 <i>H</i> ,2 <i>H</i> ,2 <i>H</i> -Perfluorooctane sulfonic acid (6:2 FTS) | 5.75 | 427.17 | 407.18 | 80.71 |
| 28. Perfluorooctanoic acid (PFOA) | 5.86 | 413.10 | 368.96 | 168.90 |
| 29. 9-Chlorohexadecafluoro-3-oxanonane-1-sulfonic acid (9Cl-PF30NS) | 5.88 | 530.78 | 350.85 | 82.96 |
| 30. Perfluorooctanesulfonic acid (PFOS) | 5.96 | 499.03 | 79.92 | 98.90 |
| 31. Perfluorononanesulfonic acid (PFNS) | 6.38 | 549.10 | 79.92 | 98.83 |
| 32. <i>N</i> -methyl perfluorooctanesulfonamidoacetic acid (NMeFOSAA) | 6.44 | 570.20 | 419.17 | 483.16 |
| 33. Perfluorononanoic acid (PFNA) | 6.45 | 463.10 | 419.01 | 219.02 |
| 34. <i>N</i> -ethyl perfluorooctanesulfonamidoacetic acid (NEtFOSAA) | 6.56 | 584.20 | 419.18 | 483.11 |
| 35. 11-Chloroicosadecafluoro-3-oxaundecane-1-sulfonic acid (11Cl-PF30UdS) | 6.56 | 630.78 | 450.80 | 82.95 |
| 36. Perfluorodecanesulfonic acid (PFDS) | 6.77 | 599.17 | 79.98 | 98.83 |
| 37. Perfluorodecanoic acid (PFDA) | 7.03 | 513.17 | 469.16 | 219.06 |
| 38. Perfluoroundecanesulfonic acid (PFUdS) | 7.12 | 648.73 | 79.94 | 98.94 |
| 39. 1 <i>H</i> ,1 <i>H</i> ,2 <i>H</i> ,2 <i>H</i> -Perfluorodecane sulfonic acid (8:2 FTS) | 7.22 | 527.17 | 507.16 | 80.83 |
| 40. Perfluorododecanesulfonic acid (PFDoS) | 7.44 | 698.77 | 79.95 | 98.94 |
| 41. Perfluoroundecanoic acid (PFUnA) | 7.60 | 563.23 | 519.24 | 269.07 |
| 42. Perfluorotridecanesulfonic acid (PFTrDS) | 7.73 | 748.73 | 79.94 | 98.94 |
| 43. Perfluorododecanoic acid (PFDoA) | 8.23 | 613.23 | 569.19 | 169.06 |
| 44. Perfluorotridecanoic acid (PFTrDA) | 8.99 | 663.23 | 619.21 | 169.06 |
| 45. Perfluorotetradecanoic acid (PFTeDA) | 9.83 | 712.67 | 668.69 | 168.94 |

Column Ultra Inert IBD (cat. # 9175312-T)
Dimensions: 100 mm x 2.1 mm ID
Particle Size: 3.0 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:methanol, 0.5% acetic acid
Conc.: 500 ng/L (ppt)
Inj. Vol.: 45 µL
Mobile Phase
A: Water, 5mM ammonium formate, 0.1% formic acid
B: Acetonitrile

| Time (min) | Flow (mL/min) | %A | %B |
|------------|---------------|----|----|
| 0.00 | 0.4 | 50 | 50 |
| 7.00 | 0.4 | 5 | 95 |
| 10.00 | 0.4 | 5 | 95 |
| 10.01 | 0.4 | 50 | 50 |
| 12.00 | 0.4 | 50 | 50 |

Max Pressure: 320 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 500 ppt standard solution was prepared in 250 µL reverse osmosis water in a 700 µL polypropylene HPLC vial followed by mixing with 250 µL of methanol containing 1% acetic acid. The vial was capped with polyethylene caps.
Notes The confirmation ion peaks were not shown in the chromatogram.

A PFAS delay column (cat # 27854) was installed before the injection.

For the chromatograms of perfluoroalkyl carboxylic acids and perfluoroalkyl sulfonic acids, the peak numbers correspond to the carbon chain lengths of the PFAS compounds.