Novel PFAS Discovery – Sequential Sampling coupled with TOFMS

Environmental Science & Technology

Identification of Novel Perfluoroalkyl Ether Carboxylic Acids (PFECAs) and Sulfonic Acids (PFESAs) in Natural Waters Using Accurate Mass Time-of-Flight Mass Spectrometry (TOFMS)

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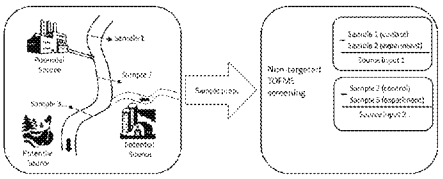
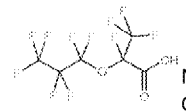


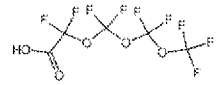
Table 1. Accurate Mass of Polyfluorinated Compounds and In-Source Artifacts Found in Extracted Water Samples

number	formula	CAS no.	name	$[M]^a$	$[M-H]^+$ m/z	$[2M-2H+Na]^+$ m/z	$[2M-H]^+$ m/z
Monoether PFECAs							
1	$C_4HF_7O_3$			179.9846	178.9773	380.9438	358.9619
2	$C_6HF_9O_3$			329.9813	328.9740	480.9372	458.9553
3	$C_6HF_9O_3$	863090-89-5		279.9782	278.9709	580.9310	558.9491
4	$C_8HF_{13}O_3$	13252-13-6	undecafluoro-2-methyl-3-oxahexanoic acid	329.9750	328.9677	680.9247	658.9427
5	$C_8HF_{13}O_3$			379.9718	378.9645	780.9182	758.9363
6	$C_8HF_{13}O_3$			429.9686	428.9613	880.9118	858.9299
Polyether PFECAs							
7	$C_7HF_{14}O_3$	39492-91-6	perfluoro-3,5,7,9,11-pentaoxadodecanoic acid	445.9515	442.9442	888.8776	886.8957
8	$C_6HF_{12}O_6$	39491-90-5	perfluoro-3,5,7,9-butaoxadecanoic acid	377.9598	376.9525	776.8942	754.9123
9	$C_5HF_9O_5$	39492-89-2	perfluoro-3,5,7-propaoxaoctanoic acid	311.9681	310.9608	644.9108	622.9289
10	$C_4HF_7O_4$	39492-88-4	perfluoro-3,5-dioxahexanoic acid	245.9764	244.9691	512.9274	490.9455
PFESAs							
11	$C_4HF_{14}O_3S$	66796-30-3[b]		445.9337	442.9264		
12	$C_4H_2F_{14}O_3S$			463.9399	462.9326		

Example Structures



Monoether (6): GenX



polyethers (4):