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Method Summary

The Determination of selected PFAS in water by LC-MS/MS.

Scope and Range

PFAS are surfactants with many industrial uses, particularly in the production of PTFE and in coatings for paper. Historically they have seen use in foaming agents, particularly aqueous film-forming foams (AFFF) used in firefighting. The release of some of these compounds into the environment is now under regulation.

Perfluoroalkyl carbo	xylic Acids (PFCA)	CAS	LOD (ng/L)
PFBA ^{2, 3}	perfluoro-n-butanoic acid	375-22-4	<2
PFPA ^{2, 3}	perfluoro-n-pentanoic acid	2706-90-3	<1
PFHxA ^{2, 3}	perfluoro-n-hexanoic acid	307-24-4	<1
PFHpA ^{2, 3}	perfluoro-n-heptanoic acid	375-85-9	<1
PFOA ^{2, 3}	perfluoro-n-octanoic acid	335-67-1	< 0.65
PFNA ^{2, 3}	perfluoro-n-nonanoic acid	375-95-1	<1
PFDA ^{2, 3}	perfluoro-n-decanoic acid	335-76-2	<2
PFUnA ^{2, 3}	perfluoro-n-undecanoic acid	2058-94-8	<2
PFDoA ^{2, 3}	perfluoro-n-dodecanoic acid	307-55-1	<2
PFTrDA ^{2, 3}	perfluoro-n-tridecanoic acid	72629-94-8	<3
PFTeA ³	perfluoro-n-tetradecanoic acid	376-06-7	<1
PFHxDA ³	perfluoro-n-hexadecanoic acid	67905-19-5	<1
PFODA ³	perfluoro-n-octadecanoic acid	16517-11-6	<1
Perfluoroalkylsulfona	ates#(PFSA)		•
PFBS ^{2, 3}	perfluoro-1-butanesulfonate	375-73-5	<1
PFPeS ^{2, 3}	perfluoro-1-pentanesulfonate	2706-91-4	<1
PFHxS ^{1,2,3}	perfluoro-1-hexanesulfonate	355-46-4	<1
PFHpS ^{2, 3}	perfluoro-1-heptanesulfonate	375-92-8	<1
PFOS ^{1,2,3}	perfluoro-1-octanesulfonate	1763-23-1	< 0.65
PFNS ^{2, 3}	perfluoro-1-nonanesulfonate	68259-12-1	<1
PFDS ^{2, 3}	perfluoro-1-decanesulfonate	335-77-3	<2
PFUnDS ^{2, 3}	perfluoro-1-undecanesulfonate	749786-16-1	<2
PFDoS ^{2, 3}	perfluoro-1-dodecanesulfonate	79780-39-5	<2
PFTrDS ²	perfluoro-1-tridecanesulfonate	791563-89-8	<2
Fluorotelomer Sulfor	nates (X:2 FTS)		-
4:2 FTS ³	4:2 fluorotelomer sulfonate	757124-72-4	<1
6:2 FTS ³	6:2 fluorotelomer sulfonate	27619-97-2	<1
8:2 FTS ³	8:2 fluorotelomer sulfonate	39108-34-4	<2
Perfluoroethylcycloh	exanesulfonate (PFECHS)	-	-
PFecHS ³	perfluoro-4-ethylcyclohexanesulfonate	646-83-3	<1
	•	•	•

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Perfluorooctanesulfonamides (FASA)		CAS	LOD (ng/L)
FBSA ³	perfluoro-1-butanesulfonamide	30334-69-1	<2
FHxSA ³	perfluoro-1-hexanesulfonamide	41997-13-1	<1
PFOSA ³	perfluoro-1-octanesulfonamide	754-91-6	<1
N-MeFOSA ³	N-methylperfluoro-1-octanesulfonamide	31506-32-8	<1
N-EtFOSA ³	N-ethylperfluoro-1-octanesulfonamide	4151-50-2	<1
Perfluoroalkanesulfo	namidoethanols (FASE)		
MeFOSE ³	2-(N-methylperfluoro-1-octanesulfonamido)ethanol	24448-09-7	<10
EtFOSE ³	2-(N-ethylperfluoro-1-octanesulfonamido)ethanol	1691-99-2	<10
Perfluorooctanesulfo	onamidoacetic Acids (FOSAA)		
MeFOSAA ³	N-methylperfluoro-1-octanesulfonamidoacetic acid	2355-31-9	<2
EtFOSAA ³	N-ethylperfluoro-1-octanesulfonamidoacetic acid	2991-50-6	<2
Chloroperfluoroalky	Ether Sulfonates (CI-PFESA)		•
9CI-PF3ONS ³	9-chlorohexadecafluoro-3-oxanonane-1-sulfonate	756426-58-1	<1
11Cl-PF3OUdS ³	1-chloroeicosafluoro-3-oxaundecane-1-sulfonate	763051-92-9	<2
Fluorotelomer Carbo	xylic Acids (n:3 FTCA)		•
3:3 FTCA ³	3-perfluoropropyl propanoic acid	356-02-5	<5
5:3 FTCA ³	3-perfluoropentyl propanoic acid	914637-49-3	<5
7:3 FTCA ³	3-perfluoroheptyl propanoic acid	812-70-4	<5
Per- and Polyfluoroa	lkyl Ether Carboxylic Acids (PFECA)		•
HFPO-DA ³	2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)-propanoic acid (GenX)	13252-13-6	<2
HFPO-TA ³	perfluoro-2,5-dimethyl-3,6-dioxanonanoic acid	13252-14-7	<5
ADONA ³	dodecafluoro-3H-4,8-dioxanonanoate	919005-14-4	<1
PFMOPrA ³	perfluoro-4-oxapentanoic acid	377-73-1	<1
PFMOBA ³	perfluoro-5-oxahexanoic acid	863090-89-5	<1
NFDHA ³	perfluoro-3,6-dioxaheptanoic acid	151772-58-6	<3
Perfluoroalkyl Ether	Sulfonates (PFESA)		
PFEESA ³	perfluoro(2-ethoxyethane)sulfonate	113507-82-7	<1
Cationic/Zwitterionic	: PFAS		
N-CMAmP-6:2FOSA	Fluorotelomer sulfonamide alkylbetaine (6:2 FTAB)	34455-29-3	<10
Total PFAS EU 20	(sum of selected PFCA and PFSA)	_	<20
Total PFAS 47	(sum of 47 selected PFAS)	-	<90
Total Identified PFAS	(sum of all detected PFAS)	-	<90
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Table 1 List of per- and polyfluorinated compounds contained within suite and associated limits of detection.

- The listed CAS numbers refer to the parent perfluoroalkylsulfonic acid. It should be noted that the method detects the pefluoroalkylsulfonate base anion which may derive from a range of

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substances, such as the parent acid and salts of the acid.

- 1 Calibration standard contains both linear and branched components
- 2 Compound included in "Total PFAS EU 20"
- 3 Compound included in "Total PFAS DWI 47"

References

EPA Method 1633 - Analysis of Per- and Polyyfluoroalkyl Substances (PFAS) in Aqueous, Solid, Biosolid, and Tissue Samples by LC-MS/MS, January 2024. EPA document EPA 821-R-24-001

Principle

Water samples which are suspected of containing per- and/or polyfluoroalkyl substances are extracted using solid phase extraction (SPE) and analysed by liquid chromatography coupled with a triple quadrupole mass spectrometer (LC-MS/MS). The identification of each analyte is confirmed by retention time combined with one or two mass transitions.

The standards used for calibration of PFOS and PFHxS contain both linear and branched components, so all are integrated when quantitating these compounds. All other compounds are quantified for the linear component only.

Holding times are set at 28 days with the following caveats:

Certain perfluorooctane sulfonamide ethanols (MeFOSE and EtFOSE) have been shown to convert to perfluorooctane sulfonamidoacetic acids (MeFOSAA and EtFOSAA). The extent of such transformation is matrix and time dependant therefore the results are indicative of levels present at the time of analysis.

Interferences

Extracted samples may contain interferences from other compounds contained within the sample matrix. Using the principles of MS/MS, many of these interferences will be eliminated. However, there may be occasions when interferences from non-target compounds arise from similar precursor and product ions. In these cases, reported limits of detection may be raised.