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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.

PFBA ^{2,3} perfluoro-n-butanoic acid 375-22.4 <2	Perfluoroalkyl carboxylic Acids (PFCA)		CAS	LOD (ng/L)		
PFPA ^{2,3} perfluoron-pentanoic acid 2706-90.3 <1	PFBA ^{2, 3}	perfluoro-n-butanoic acid	375-22-4	<2		
PFHxA ^{2,3} perfluoro-n-hexanoic acid 307-24.4 <1 PFHpA ^{2,3} perfluoro-n-heptanoic acid 375-85-9 <1	PFPA ^{2, 3}	perfluoro-n-pentanoic acid	2706-90-3	<1		
PFHpA ^{2.3} perfluoro-n-heptanoic acid 375-85-9 <1 PFOA ^{2.3} perfluoro-n-octanoic acid 335-67-1 <0.65	PFHxA ^{2, 3}	perfluoro-n-hexanoic acid	307-24-4	<1		
PFOA ^{2,3} perfluoro-n-octanoic acid 335-67-1 <0.65 PFNA ^{2,3} perfluoro-n-onanoic acid 375-95-1 <1	PFHpA ^{2, 3}	perfluoro-n-heptanoic acid	375-85-9	<1		
PFNA ^{2.3} perfluoro-n-nonanoic acid 375-95-1 <1 PFDA ^{2.3} perfluoro-n-decanoic acid 335.76-2 <2	PFOA ^{2, 3}	perfluoro-n-octanoic acid	335-67-1	<0.65		
PFDA ^{2.3} perfluoro-n-decanoic acid 335.76-2 <2 PFUnA ^{2.3} perfluoro-n-undecanoic acid 2058.94.8 <2	PFNA ^{2, 3}	perfluoro-n-nonanoic acid	375-95-1	<1		
PFUnA ^{2,3} perfluoron-undecanoic acid 2058-94-8 <2 PFDoA ^{2,3} perfluoron-dodecanoic acid 307-55-1 <2	PFDA ^{2, 3}	perfluoro-n-decanoic acid	335-76-2	<2		
PFDoA ^{2,3} perfluoro-n-dodecanoic acid 307-55-1 <2 PFTrDA ^{2,3} perfluoro-n-tridecanoic acid 72629-94-8 <3	PFUnA ^{2, 3}	perfluoro-n-undecanoic acid	2058-94-8	<2		
PFTrDA ^{2,3} perfluoro-n-tridecanoic acid 72629-94-8 <3 PFTeA ³ perfluoro-n-tetradecanoic acid 376-06-7 <1	PFDoA ^{2, 3}	perfluoro-n-dodecanoic acid	307-55-1	<2		
PFTeA ³ perfluoro-n-tetradecanoic acid 376-06-7 <1 PFHxDA ³ perfluoro-n-hexadecanoic acid 67905-19-5 <1	PFTrDA ^{2, 3}	perfluoro-n-tridecanoic acid	72629-94-8	<3		
PFHxDA ³ perfluoro-n-hexadecanoic acid 67905-19-5 <1 PFODA ³ perfluoro-n-octadecanoic acid 16517-11-6 <1	PFTeA ³	perfluoro-n-tetradecanoic acid	376-06-7	<1		
PFODA ³ perfluoro-n-octadecanoic acid 16517-11-6 <1 Perfluoroalkylsulfonate*'(PFSA) <t< td=""><th>PFHxDA³</th><td>perfluoro-n-hexadecanoic acid</td><td>67905-19-5</td><td><1</td></t<>	PFHxDA ³	perfluoro-n-hexadecanoic acid	67905-19-5	<1		
Perfluoroalkylsulfonates* (PFSA) PFBS ^{2,3} perfluoro-1-butanesulfonate 375-73-5 <1	PFODA ³	perfluoro-n-octadecanoic acid	16517-11-6	<1		
PFBS ^{2,3} perfluoro-1-butanesulfonate 375-73-5 <1	Perfluoroalkylsulfonate	es [#] (PFSA)				
PFPeS ^{2,3} perfluoro-1-pentanesulfonate 2706-91-4 <1 PFHxS ^{1,2,3} perfluoro-1-hexanesulfonate 355-46-4 <1	PFBS ^{2, 3}	perfluoro-1-butanesulfonate	375-73-5	<1		
PFHxS ^{1,2,3} perfluoro-1-hexanesulfonate 355-46-4 <1 PFHpS ^{2,3} perfluoro-1-heptanesulfonate 375-92-8 <1	PFPeS ^{2, 3}	perfluoro-1-pentanesulfonate	2706-91-4	<1		
PFHpS ^{2.3} perfluoro-1-heptanesulfonate 375-92-8 <1 PFOS ^{1.2.3} perfluoro-1-octanesulfonate 1763-23-1 <1	PFHxS ^{1,2,3}	perfluoro-1-hexanesulfonate	355-46-4	<1		
PFOS ^{1,2,3} perfluoro-1-octanesulfonate 1763-23-1 <1 PFNS ^{2,3} perfluoro-1-nonanesulfonate 68259-12-1 <1	PFHpS ^{2, 3}	perfluoro-1-heptanesulfonate	375-92-8	<1		
PFNS ^{2,3} perfluoro-1-nonanesulfonate 68259-12-1 <1 PFDS ^{2,3} perfluoro-1-decanesulfonate 335-77-3 <2	PFOS ^{1,2,3}	perfluoro-1-octanesulfonate	1763-23-1	<1		
PFDS ^{2,3} perfluoro-1-decanesulfonate 335-77-3 <2 PFUnDS ^{2,3} perfluoro-1-undecanesulfonate 749786-16-1 <2	PFNS ^{2, 3}	perfluoro-1-nonanesulfonate	68259-12-1	<1		
PFUnDS ^{2,3} perfluoro-1-undecanesulfonate 749786-16-1 <2 PFDoS ^{2,3} perfluoro-1-dodecanesulfonate 79780-39-5 <2	PFDS ^{2, 3}	perfluoro-1-decanesulfonate	335-77-3	<2		
PFDoS ^{2.3} perfluoro-1-dodecanesulfonate 79780-39-5 <2 PFTrDS ² perfluoro-1-tridecanesulfonate 174675-49-1 <2	PFUnDS ^{2, 3}	perfluoro-1-undecanesulfonate	749786-16-1	<2		
PFTrDS ² perfluoro-1-tridecanesulfonate 174675-49-1 <2 Fluorotelomer Sulfonates (X:2 FTS) 4:2 FTS ³ 4:2 fluorotelomer sulfonate 757124-72-4 <1	PFDoS ^{2, 3}	perfluoro-1-dodecanesulfonate	79780-39-5	<2		
Fluorotelomer Sulfonates (X:2 FTS) 4:2 FTS ³ 4:2 fluorotelomer sulfonate 757124-72-4 <1	PFTrDS ²	perfluoro-1-tridecanesulfonate	174675-49-1	<2		
4:2 FTS ³ 4:2 fluorotelomer sulfonate 757124-72-4 <1	Fluorotelomer Sulfona	Fluorotelomer Sulfonates (X:2 FTS)				
6:2 FTS ³ 6:2 fluorotelomer sulfonate 27619-97-2 <1 8:2 FTS ³ 8:2 fluorotelomer sulfonate 39108-34-4 <2	4:2 FTS ³	4:2 fluorotelomer sulfonate	757124-72-4	<1		
8:2 FTS ³ 8:2 fluorotelomer sulfonate 39108-34-4 <2 Perfluoroethylcyclohexanesulfonate (PFECHS) PFecHS ³ perfluoro-4-ethylcyclohexanesulfonate 13252-14-7 <1	6:2 FTS ³	6:2 fluorotelomer sulfonate	27619-97-2	<1		
Perfluoroethylcyclohexanesulfonate (PFECHS) PFecHS ³ perfluoro-4-ethylcyclohexanesulfonate 13252-14-7 <1	8:2 FTS ³	8:2 fluorotelomer sulfonate	39108-34-4	<2		
PFecHS ³ perfluoro-4-ethylcyclohexanesulfonate 13252-14-7 <1	Perfluoroethylcyclohexanesulfonate (PFECHS)					
	PFecHS ³	perfluoro-4-ethylcyclohexanesulfonate	13252-14-7	<1		

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Perfluorooctanesulfo	onamides (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		
Perfluorooctanesulfonamidoacetic Acids (FOSAA)					
MeFOSAA ³	N-methylperfluoro-1-octanesulfonamidoacetic acid	2355-31-9	<2		
EtFOSAA ³	N-ethylperfluoro-1-octanesulfonamidoacetic acid	2991-50-6	<2		
Chloroperfluoroalkyl 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	<2		
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		
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		

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

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- 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 Draft Method 1633 - Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous, Solid, Biosolid, and Tissue Damples by LC-MS/MS, August 2021. EPA document EPA 821-D-21-001.

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 14 days with the following caveat:

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.