

Supplementary Material (ESI) for Journal of Environmental Monitoring

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S1: Analytes, acronyms, formula, supplier, purity, precursor and product ion, and corresponding internal standard

Substance	Acronym	Formula	Supplier and purity (%)	Precursor/Product ion	Corresponding IS
Perfluorobutane sulfonate	PFBS	C ₄ F ₉ SO ₂ O ⁻	Fluka (97)	298.877/79.8	[¹⁸ O ₂]-PFHxS
Perfluoropentane sulfonate	PFPS	C ₅ F ₁₁ SO ₂ O ⁻	n.a.	348.939/79.8	[¹⁸ O ₂]-PFHxS
Perfluorohexane sulfonate	PFHxS	C ₆ F ₁₃ SO ₂ O ⁻	Fluka (98)	398.939/79.8	[¹⁸ O ₂]-PFHxS
Perfluorheptane sulfonate	PFHpS	C ₇ F ₁₅ SO ₂ O ⁻	Well. Lab. (>98)	449.034/79.3	[¹³ C ₄]-PFOS
Perfluorocotane sulfonate	PFOS	C ₈ F ₁₇ SO ₂ O ⁻	Well. Lab. (>98)	498.971/97.7	[¹³ C ₄]-PFOS
Perfluorononane sulfonate	PFNS	C ₉ F ₁₉ SO ₂ O ⁻	n.a.	548.926/79.8	[¹³ C ₄]-PFOS
Perfluorodecane sulfonate	PFDS	C ₁₀ F ₂₁ SO ₂ O ⁻	Well. Lab. (>98)	598.896/79.5	[¹³ C ₄]-PFOS
6:2 fluorotemomer sulfonate	6:2 FTS	C ₆ F ₁₃ C ₂ H ₄ SO ₃	ABCR (98)	426.925/406.7	[¹³ C ₄]-PFOS
Perfluorobutanoic acid	PFBA	C ₃ F ₇ COOH	ABCR (98)	112.900/168.7	[¹³ C ₄]-PFOSI
Perfluoropentanoic acid	PFPeA	C ₄ F ₉ COOH	Alfa Aesar (98)	262.825/218.9	[¹³ C ₄]-PFBA
Perfluorohexanoic acid	PFHxA	C ₅ F ₁₁ COOH	Fluka (97)	312.934/268.8	[¹³ C ₂]-PFHxA
Perfluoroheptanoic acid	PFHpA	C ₆ F ₁₃ COOH	Lanc. Syn. (98)	362.950/318.9	[¹³ C ₂]-PFHxA
Perfluorooctanoic acid	PFOA	C ₇ F ₁₄ COOH	Lanc. Syn. (95)	412.987/368.9	[¹³ C ₄]-PFOA
Perfluorononanoic acid	PFNA	C ₈ F ₁₅ COOH	Lanc. Syn. (97)	462.908/418.9	[¹³ C ₄]-PFOA
Perfluorodecanoic acid	PFDA	C ₉ F ₁₇ COOH	Lanc. Syn. (97)	512.876/469.0	[¹³ C ₅]-PFNA
Perfluoroundecanoic acid	PFUnDA	C ₁₀ F ₁₉ COOH	ABCR (96)	562.865/519.0	[¹³ C ₂]-PFDA
Perfluorododecanoic acid	PFDoDA	C ₁₁ F ₂₁ COOH	Alfa Aesar (96)	612.991/568.9	[¹³ C ₂]-PFUnDA
Perfluorotridecanoic acid	PFTriDA	C ₁₂ F ₂₃ COOH	Well. Lab. (>98)	663.094/618.9	[¹³ C ₂]-PFDoDA
Perfluorotetradecanoic acid	PFTeDA	C ₁₃ F ₂₅ COOH	Alfa Aesar (96)	713.036/669.0	[¹³ C ₂]-PFDoDA
Perfluorotridecanoic acid	PFPDA	C ₁₄ F ₂₇ COOH	n.a.	762.980/718.9	[¹³ C ₂]-PFDoDA
Perfluorohexadecanoic acid	PFHxDA	C ₁₅ F ₂₉ COOH	Alfa Aesar (96)	812.840/769.1	[¹³ C ₂]-PFDoDA
Perfluoroheptadecanoic acid	PFHpDA	C ₁₆ F ₃₁ COOH	n.a.	862.980/818.9	[¹³ C ₂]-PFDoDA
Perfluorooctadecanoic acid	PFOcDA	C ₁₇ F ₃₃ COOH	Alfa Aesar (96)	912.870/869.0	[¹³ C ₂]-PFDoDA
Perfluoro-3,7-bis(trifluoromethyl)-octanoic acid	3,7m ₂ -PFOA	C ₈ F ₁₉ COOH	Alfa Aesar (97)	512.885/468.9	[¹³ C ₄]-PFOA
Perfluorohexylphosphonic acid	PFHxA	C ₆ F ₁₃ PO(OH) ₂	Well. Lab. (>98)	399.000/78.8	[¹³ C ₄]-PFOS
Perfluorooctylphosphonic acid	PFOPA	C ₈ F ₁₇ PO(OH) ₂	Well. Lab. (>98)	499.000/78.8	[¹³ C ₄]-PFOS
Perfluorodecylphosphonic acid	PFDPDA	C ₁₀ F ₂₁ PO(OH) ₂	Well. Lab. (>98)	599.100/78.8	[¹³ C ₄]-PFOS
Perfluorooctane sulfonamid	PFOSA	C ₈ F ₁₇ SO ₂ NH ₂	ABCR (97)	497.896/77.9	[¹³ C ₄]-PFOS
N-methylperfluorobutane sulfonamidoethanol	MEFBSE	C ₄ F ₉ SO ₂ N(CH ₃)C ₂ H ₄ OH	3M (n.a.)	416.047/59.0	[¹³ C ₄]-PFOS
2-perfluorohexylethanoic acid	FHEA	C ₆ F ₁₃ CH ₂ COOF	Well. Lab. (>98)	376.945/292.8	[¹³ C]-CFHEA
2-perfluorooctylethanoic acid	FOEA	C ₈ F ₁₇ CH ₂ COOH	Well. Lab. (>98)	476.909/392.9	[¹³ C]-FOEA
2-perfluorodecylethanoic acid	FDEA	C ₁₀ F ₂₁ CH ₂ COOH	Well. Lab. (>98)	577.011/493.0	[¹³ C]-FDEA
2H-perfluoro-2-octenoic acid	FHUEA	C ₆ F ₁₂ CHCOOH	Well. Lab. (>98)	356.885/293.0	[¹³ C]-FHUEA
2H-perfluoro-2-decenoic acid	FOUEA	C ₈ F ₁₆ CHCOOH	Well. Lab. (>98)	456.803/292.8	[¹³ C]-FOUEA
2H-perfluoro-2-dodecenoic acid	FDUEA	C ₁₀ F ₂₀ CHCOOH	Well. Lab. (>98)	556.973/493.1	[¹³ C]-FDUEA

S2: Internal standards and injection standard, acronyms, formula, supplier, purity, precursor and product ion

Internal Standard	Acronym	Formula	Supplier and purity (%)	Precursor/Product ion
Perfluoro-1-hexane- ¹⁸ O ₂]sulfonate	[¹⁸ O ₂]-PFHxS	C ₆ F ₁₃ S[¹⁸ O ₂]O ⁻	Well. Lab. (>98)	402.981/83.9
Perfluoro-1-[1,2,3,4- ¹³ C ₄]octanesulfonate	[¹³ C ₄]-PFOS	C ₄ F ₉ [1,2,3,4- ¹³ C ₄]-F ₈ SO ₂ O ⁻	Well. Lab. (>98)	502.899/79.5
Perfluoro-n-[1,2,3,4- ¹³ C ₄]butanoic acid	[¹³ C ₄]-PFBA	2,3,4- ¹³ C ₃ F ₇ ¹³ COOH	Well. Lab. (>98)	216.823/171.8
Perfluoro-n-[1,2- ¹³ C ₂]hexanoic acid	[¹³ C ₂]-PFHxA	C ₄ F ₉ [2- ¹³ C]F ₂ ¹³ COOH	Well. Lab. (>98)	314.891/269.9
Perfluoro-n-[1,2,3,4- ¹³ C ₄]octanoic acid	[¹³ C ₄]-PFOA	C ₄ F ₉ [2,3,4- ¹³ C ₃]F ₆ ¹³ COOH	Well. Lab. (>98)	416.978/371.8
Perfluoro-n-[1,2,3,4,5- ¹³ C ₅]nonanoic acid	[¹³ C ₅]-PFNA	C ₄ F ₉ [2,3,4,5- ¹³ C ₅]F ₈ ¹³ COOH	Well. Lab. (>98)	467.907/423.0
Perfluoro-n-[1,2- ¹³ C ₂]decanoic acid	[¹³ C ₂]-PFDA	C ₈ F ₁₇ ¹³ CF ₂ ¹³ COOH	Well. Lab. (>98)	514.944/469.8
Perfluoro-n-[1,2- ¹³ C ₂]undecanoic acid	[¹³ C ₂]-PFUnDA	C ₉ F ₁₉ ¹³ CF ₂ ¹³ COOH	Well. Lab. (>98)	564.959/519.8
Perfluoro-n-[1,2- ¹³ C]dodecanoin acid	[¹³ C ₂]-PFD _o DA	C ₁₀ F ₂₁ CF ₂ ¹³ COOH	Well. Lab. (>98)	614.9 ¹³ /569.9
2-perfluorohexyl-[1,2- ¹³ C ₂]ethanoic acid	[¹³ C ₂]-FHEA	C ₆ F ₁₃ CH ₂ ¹³ COOH	Well. Lab. (>98)	378.912/294.0
2-perfluorooctyl-[1,2- ¹³ C ₂]ethanoic acid	[¹³ C ₂]-FOEA	C ₈ F ₁₇ ¹³ CH ₂ ¹³ COOH	Well. Lab. (>98)	478.911/393.8
2-perfluorodecyl-[1,2- ¹³ C ₂]-FDEA	[¹³ C ₂]-FDEA	C ₁₀ F ₂₁ ¹³ CH ₂ ¹³ COOH	Well. Lab. (>98)	579.017/494.1
2H-perfluoro-[1,2- ¹³ C ₂]-2-octenoic acid	[¹³ C ₂]-FHUEA	C ₆ F ₁₂ ¹³ CH ¹³ COOH	Well. Lab. (>98)	358.907/294.0
2H-perfluoro-[1,2- ¹³ C ₂]-2-decenoic acid	[¹³ C ₂]-FOUEA	C ₈ F ₁₆ ¹³ CH ¹³ COOH	Well. Lab. (>98)	458.903/393.8
2H-perfluoro-[1,2- ¹³ C ₂]-2-dodecenoic acid	[¹³ C ₂]-FDUEA	C ₁₀ F ₂₀ ¹³ CH ¹³ COOH	Well. Lab. (>98)	558.955/494.0
N-deuterioethylperfluoro-1-octanesulfonamidoacetic acid	D5-EtFOSA A	C ₈ F ₁₇ SO ₂ N(C ₂ D ₂ C ₂ D ₃)C ₂ H ₂ CO ₂ H	Well. Lab. (>98)	589.015/418.7

S3: Recovery rates of each internal standard (IS) in the water samples.

Substance	Recovery rate
¹⁸ O ₂ -PFHXS	23.4 ± 10.6
¹³ C-PFOS	22.0 ± 13.0
¹³ C-PFBA	9.88 ± 18.5
¹³ C-PFHxA	21.4 ± 34.9
¹³ C-PFOA	27.9 ± 10.8
¹³ C-PFNA	35.1 ± 12.9
¹³ C-PFDA	23.6 ± 12.8
¹³ C-PFU _n DA	15.9 ± 11.6
¹³ C-PFDoDA	13.8 ± 10.6
¹³ C-FHEA	23.0 ± 10.9
¹³ C-FHOEA	36.1 ± 13.9
¹³ C-FDEA	16.9 ± 12.3
¹³ C-FHUEA	23.1 ± 10.3
¹³ C-FOUEA	35.6 ± 17.1
¹³ C-FDUEA	16.3 ± 12.1
mean	22.9 ± 14.1

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S4: Mass detection limits (MDL) and mass quantification limits (MQL) calculated as signal-to-noise ratio of three and ten, respectively, in pg L^{-1} for all compounds found in the water samples. PFNS is not in the list, since it was not quantified.

substance	MDL	MQL
PFHxS	9.86	32.9
PFOS	22.7	75.5
PFHxA	13.2	43.9
PFHpA	5.78	19.3
PFOA	11.8	39.4
PFNA	3.06	10.2
PFOSA	36.5	122

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S5: Concentrations of each compound found in 2 L water samples. All concentrations are in pg L^{-1} . Concentrations between MDL and MQL are shown as calculated concentrations. In the manuscript concentrations between MDL and MQL were defined as 50% MDL. (n.d. = not detected)

	PFOA	PFHpA	PFHxA	PFNS	PFOS	PFHxS	PFOSA	latitude	salinity (psu)
1	17.43	n.d.	n.d.	160.18	42.64	10.73	n.d.	67.51	34.72
2	45.87	n.d.	n.d.	74.21	45.31	n.d.	36.35	68.95	34.62
3	24.83	n.d.	n.d.	91.85	n.d.	n.d.	n.d.	69.46	34.72
4	38.90	n.d.	n.d.	51.54	49.67	n.d.	n.d.	70.39	34.65
5	61.41	n.d.	n.d.	71.68	25.36	n.d.	n.d.	70.45	36.66
6	94.90	17.01	16.66	28.65	38.62	22.81	n.d.	70.73	32.64
7	29.39	6.78	n.d.	n.d.	54.48	n.d.	n.d.	70.86	33.19
8	65.19	24.60	n.d.	34.61	n.d.	16.90	n.d.	71.57	26.21
9	49.59	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	72.03	34.61
10	53.98	9.22	n.d.	22.17	50.39	21.66	49.23	72.07	25.28
11	44.69	n.d.	n.d.	23.01	54.91	18.90	72.55	72.23	19.02
12	72.36	23.00	15.41	n.d.	n.d.	n.d.	62.24	73.02	21.45
13	85.15	19.67	n.d.	n.d.	n.d.	17.53	n.d.	73.15	29.34
14	69.47	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	73.45	33.38
15	6.70	n.d.	n.d.	n.d.	n.d.	n.d.	162.86	73.80	34.36
16	32.93	12.30	n.d.	n.d.	n.d.	n.d.	51.43	73.98	33.83
17	82.15	26.89	n.d.	n.d.	39.18	14.72	76.12	74.24	29.95
18	38.06	7.84	n.d.	n.d.	n.d.	n.d.	n.d.	74.42	33.18
19	46.29	6.56	n.d.	n.d.	n.d.	n.d.	37.37	74.63	34.41
20	12.53	n.d.	n.d.	n.d.	n.d.	n.d.	123.64	75.37	34.89
21	68.09	26.77	14.73	n.d.	n.d.	10.41	n.d.	76.15	25.70
22	19.66	n.d.	n.d.	n.d.	n.d.	n.d.	75.28	76.18	35.12
23	62.31	7.67	n.d.	n.d.	n.d.	n.d.	150.09	76.37	35.01
24	37.40	7.39	n.d.	n.d.	n.d.	n.d.	184.18	76.41	35.08
25	77.49	15.42	16.90	n.d.	n.d.	14.39	n.d.	76.47	26.65
26	54.67	n.d.	n.d.	n.d.	n.d.	n.d.	98.86	76.85	34.71
27	22.71	n.d.	n.d.	n.d.	n.d.	n.d.	130.62	77.12	34.18
28	26.65	n.d.	n.d.	n.d.	31.29	n.d.	111.89	77.22	35.00
29	46.06	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	77.41	34.78
30	119.71	23.11	33.26	n.d.	n.d.	24.12	n.d.	78.21	34.98
31	91.47	20.40	18.70	n.d.	n.d.	18.53	300.03	78.31	27.62
32	69.97	17.01	n.d.	n.d.	n.d.	26.94	99.05	79.05	28.89
33	34.85	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	79.11	34.72
34	40.44	6.14	n.d.	n.d.	n.d.	n.d.	217.91	79.94	32.26
35	48.26	20.82	n.d.	n.d.	n.d.	n.d.	41.86	80.16	28.63
36	117.07	26.76	37.72	n.d.	n.d.	n.d.	192.09	80.23	29.95
37	64.40	19.56	14.41	n.d.	n.d.	n.d.	72.31	80.31	24.57
38	57.17	19.81	17.17	n.d.	n.d.	11.94	80.31	80.43	26.51

S6: Concentrations of compounds (PFHxA, PFHpA, PFOA, PFOS, PFOSA) in $\mu\text{g L}^{-1}$.

Graphics were made with Ocean Data View 4 (<http://odv.awi.de/en>)



