Supplementary Material (ESI) for Journal of Environmental Monitoring

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	$C_4F_9SO_2O^-$	Fluka (97)	298.877/79.8	[^{18}O2]-PFHxS
Perfluoropentane sulfonate	PFPS	$C5F_{11}SO_2O^-$	n.a.	348.939/79.8	[^{18}O2]-PFHxS
Perfluorohexane sulfonate	PFHxS	$C6F_{13}SO_2O^-$	Fluka (98)	398.939/79.8	[^{18}O2]-PFHxS
Perfluorheptane sulfonate	PFHpS	$C_7F_15SO_2O^-$	Well. Lab. (>98)	449.034/79.3	[^{13}C4]-PFOS
Perfluororcotane sulfonate	PFOS	$C_8F_{17}SO_2O^-$	Well. Lab. (>98)	498.971/97.7	[^{13}C4]-PFOS
Perfluorononane sulfonate	PFNS	$C_9F_{19}SO_2O^-$	n.a.	548.926/79.8	[^{13}C4]-PFOS
Perfluorodecane sulfonate	PFDS	$C_{10}F_{21}SO_2O^-$	Well. Lab. (>98)	598.896/79.5	[^{13}C4]-PFOS
6:2 fluorotemomer sulfonate	6:2 FTS	$C_6F_{13}C_2H_4SO_3$	ABCR (98)	426.925/406.7	[^{13}C4]-PFOS
Perfluorobutanoic acid	PFBA	C3F7COOH	ABCR (98)	112.900/168.7	[^{13}C4]-PFOSI
Perfluoropentanoic acid	PFPeA	C4F9COOH	Alfa Aesar (98)	262.825/218.9	[^{13}C4]-PFBA
Perfluorohexanoic acis	PFHxA	C5F11COOH	Fluka (97)	312.934/268.8	[^{13}C2]-PFHxA
Perfluoroheptanoic acid	PFHpA	C6F^{13}COOH	Lanc. Syn. (98)	362.950/318.9	[^{13}C2]-PFHxA
Perfluorooctanoic acid	PFOA	$C_7F_{14}COOH$	Lanc. Syn. (95)	412.987/368.9	[^{13}C4]-PFOA
Perfluorononaoic acid	PFNA	$C_8F_{15}COOH$	Lanc. Syn. (97)	462.908/418.9	[^{13}C4]-PFOA
Perfluorodecanoic acid	PFDA	$C_9F_{17}COOH$	Lanc. Syn. (97)	512.876/469.0	[^{13}C5]-PFNA
Perfluoroundecanoic acid	PFUnDA	$C_{10}F_{19}COOH$	ABCR (96)	562.865/519.0	[^{13}C2]-PFDA
Perfluorododecanoic acid	PFDoDA	$C_{11}F_{21}COOH$	Alfa Aesar (96)	612.991/568.9	[^{13}C2]-PFUnDA
Perfluorortridecanoic acid	PFTriDA	$C_{12}F_{23}COOH$	Well. Lab. (>98)	663.094/618.9	[^{13}C2]PFDoDA
Perfluorotetradecanoic acid	PFTeDA	$C_{13}F_{25}COOH$	Alfa Aesar (96)	713.036/669.0	[^{13}C2]-PFDoDA
Perfluorotridecanoic acid	PFPDA	$C_{14}F_{27}COOH$	n.a.	762.980/718.9	[^{13}C2]-PFDoDA
Perfluorohexadecanoic acid	PFHxDA	$C_{15}F_{29}COOH$	Alfa Aesar (96)	812.840/769.1	[^{13}C2]-PFDoDA
Perfluoroheptadecanoic acid	PFHpDA	$C_{16}F_{31}COOH$	n.a	862.980/818.9	[^{13}C2]-PFDoDA
Perfluorooctadecanoic acid	PFOcDA	$C_{17}F_{33}COOH$	Alfa Aesar (96)	912.870/869.0	[^{13}C2]-PFDoDA
Perfluoro-3,7-bis(trifluoromethyl)-octanoic acid	3,7m$_2$-PFOA	$C_6F_{19}COOH$	Alfa Aesar (97)	512.885/468.9	[^{13}C4]-PFOA
Perfluorohexlyphosphonic acid	PFHxA	$C_6F_{13}PO(OH)_2$	Well. Lab. (>98)	399.000/78.8	[^{13}C4]-PFOS
Perfluorooctylphosphonic acid	PFOPA	$C_8F_{17}PO(OH)_2$	Well. Lab. (>98)	499.000/78.8	[^{13}C4]-PFOS
Perfluorodecylphosphonic acid	PFDPA	$C_{10}F_{21}PO(OH)_2$	Well. Lab. (>98)	599.100/78.8	[^{13}C4]-PFOS
Perfluorooctane sulfonamid	PFOSA	$C_8F_{17}SO_2NH_2$	ABCR (97)	497.896/77.9	[^{13}C4]-PFOS
N-methylperfluorobutane sulfonamidoethanol	MEFBSE	$C_4F_9SO_2N(CH_3)C_2H_4OH$	3M (n.a.)	416.047/59.0	[^{13}C4]-PFOS
2-perfluorohexylethanoic acid	FHEA	$C_6F_{13}CH_2COOF$	Well. Lab. (>98)	376.945/292.8	[^{13}C]-CFHEA
2-perfluorooctylethanoic acid	FOEA	$C_8F_{17}CH_2COOH$	Well. Lab. (>98)	476.909/392.9	[^{13}C]-FOEA
2-perfluorodecylethanoic acid	FDEA	$C_10F_{21}CH_2COOH$	Well. Lab. (>98)	577.011/493.0	[^{13}C]-FDEA
2H-perfluoro-2-octenoic acid	FHUEA	$C_6F_{12}CHCOOH$	Well. Lab. (>98)	356.885/293.0	[^{13}C]-FHUEA
2H-perfluoro-2-decenoic acid	FOUEA	$C_8F_{16}CHCOOH$	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	$C_6F_{13}S[^{18}O_2]O^-$	Well. Lab. (>98)	402.981/83.9
Perfluoro-1-[1,2,3,4-$^{13}C_4$]octanesulfonate	[$^{13}C_4$]-PFOS	$C_4F_9[1,2,3,4\text{-}^{13}C_4]\text{-}F_8SO_2O^-$	Well. Lab. (>98)	502.899/79.5
Perfluoro-n-[1,2,3,4-$^{13}C_4$]butanoic acid	[$^{13}C_4$]-PFBA	$2,3,4\text{-}^{13}C_3]F_7{}^{13}COOH$	Well. Lab. (>98)	216.823/171.8
Perfluoro-n-[1,2-$^{13}C_2$]hexanoic acid	[$^{13}C_2$]-PFHxA	$C_4F_9[2\text{-}^{13}C]F_2{}^{13}COOH$	Well. Lab. (>98)	314.891/269.9
Perfluoro-n-[1,2,3,4-$^{13}C_4$]octanoic acid	[$^{13}C_4$]-PFOA	$C_4F_9[2,3,4\text{-}^{13}C_3]F_6{}^{13}COOH$	Well. Lab. (>98)	416.978/371.8
Perfluoro-n-[1,2,3,4,5-$^{13}C_5$]nonanoic acid	[$^{13}C_5$]-PFNA	$C_4F_9[2,3,4,5\text{-}^{13}C_5]F_8{}^{13}COOH$	Well. Lab. (>98)	467.907/423.0
Perfluoro-n-[1,2-$^{13}C_2$]decanoic acid	[$^{13}C_2$]-PFDA	$C_8F_{17}{}^{13}CF_2{}^{13}COOH$	Well. Lab. (>98)	514.944/469.8
Perfluoro-n-[1,2-$^{13}C_2$]undecanoic acid	[$^{13}C_2$]-PFUnDA	$C_9F_{19}{}^{13}CF_2{}^{13}COOH$	Well. Lab. (>98)	564.959/519.8
Perfluoro-n-[1,2-^{13}C]dodecanoin acid	[$^{13}C_2$]-PFDoDA	$C_{10}F_{21}CF_2{}^{13}COOH$	Well. Lab. (>98)	614.9^{13}/569.9
2-perfluorohexyl-[1,2-^{13}C2]ethanoic acid	[$^{13}C_2$]-FHEA	$C_6F_{13}CH_2{}^{13}COOH$	Well. Lab. (>98)	378.912/294.0
2-perfluorooctyl-[1,2-^{13}C2]ethanoic acid	[$^{13}C_2$]-FOEA	$C_8F_{17}{}^{13}CH_2{}^{13}COOH$	Well. Lab. (>98)	478.911/393.8
2-perfluorodecyl-[1,2-^{13}C2]-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	$C_6F_{12}{}^{13}CH^{13}COOH$	Well. Lab. (>98)	358.907/294.0
2H-perfluoro-[1,2-$^{13}C_2$]-2-decenoic acid	[$^{13}C_2$]-FOUEA	$C_8F_{16}{}^{13}CH^{13}COOH$	Well. Lab. (>98)	458.903/393.8
2H-perfluoro-[1,2-$^{13}C_2$]-2-dodecanoic 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-EtFOSAA	$C_8F_{17}SO_2N(C_2D_2C_2D_3)C_2H_2CO_2H$	Well. Lab. (>98)	589.015/418.7

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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-PFUnDA	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

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

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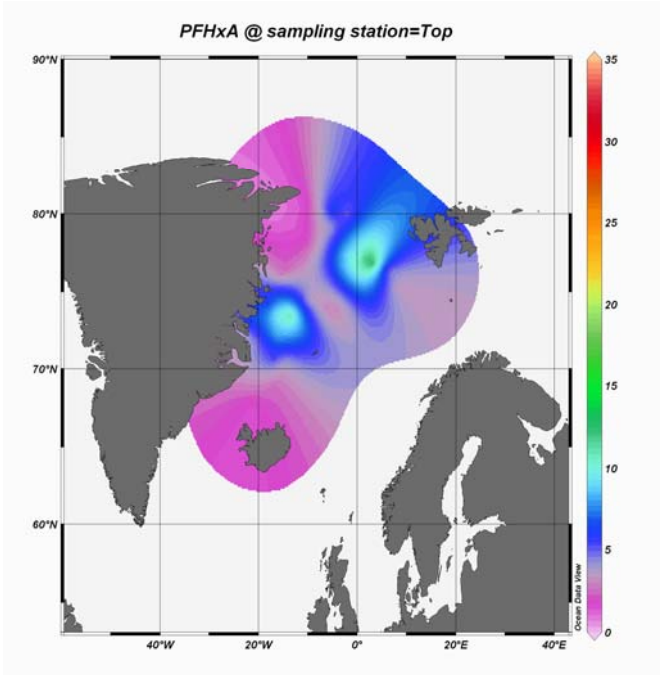
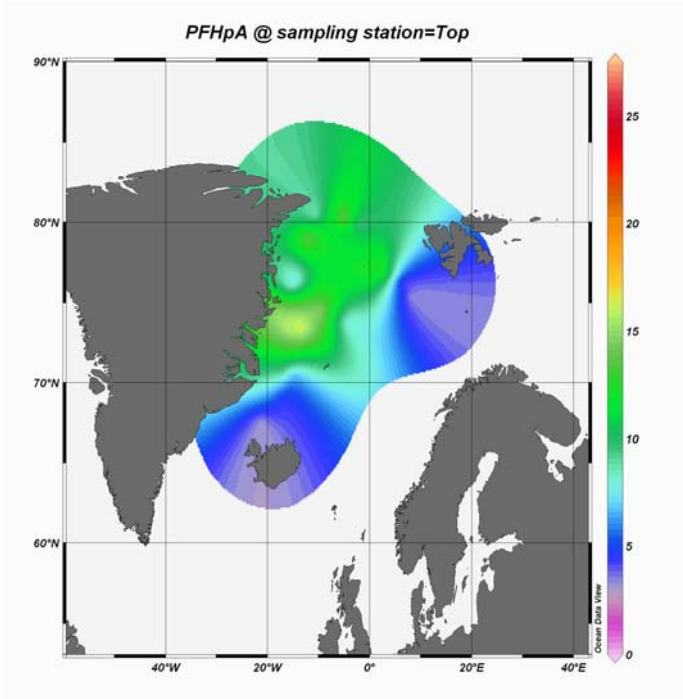
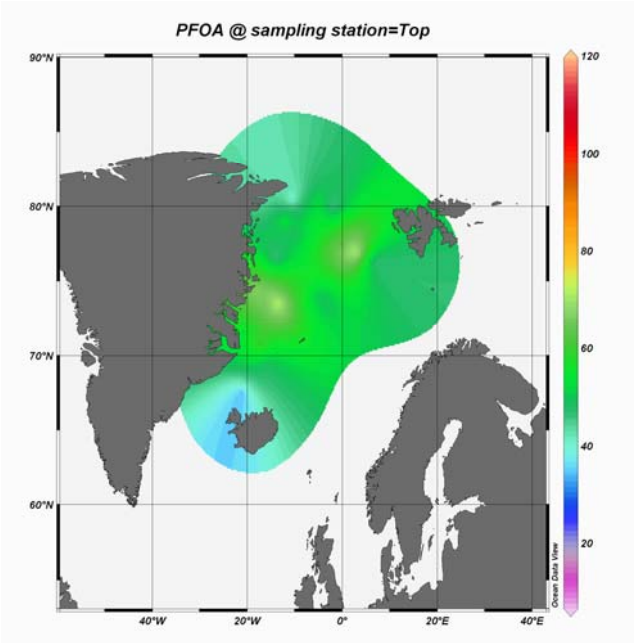
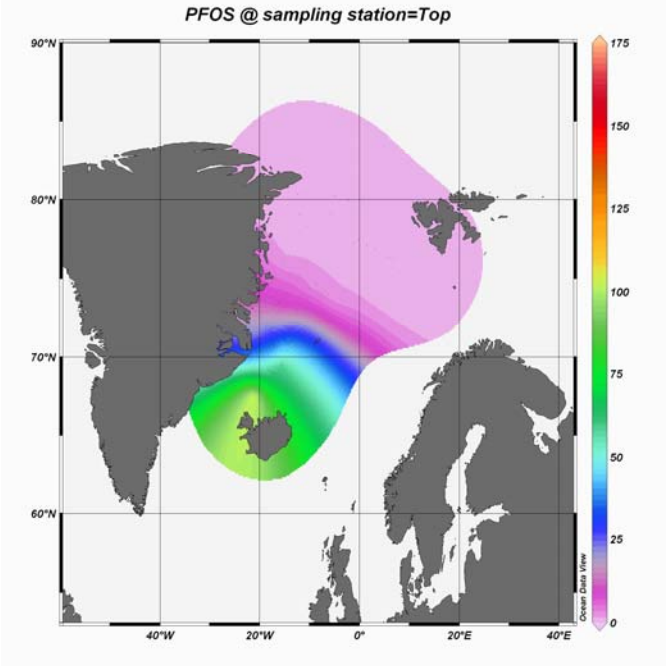
S6: Concentrations of compounds (PFHxA, PFHpA, PFOA, PFOS, PFOSA) in pg L^{-1}. Graphics were made with Ocean Data View 4 (http://odv.awi.de/en)









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