Accessory publication

Perfluorinated compounds in marine surface waters: data from the Baltic Sea and methodological challenges for future studies

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Information on the Baltic Sea

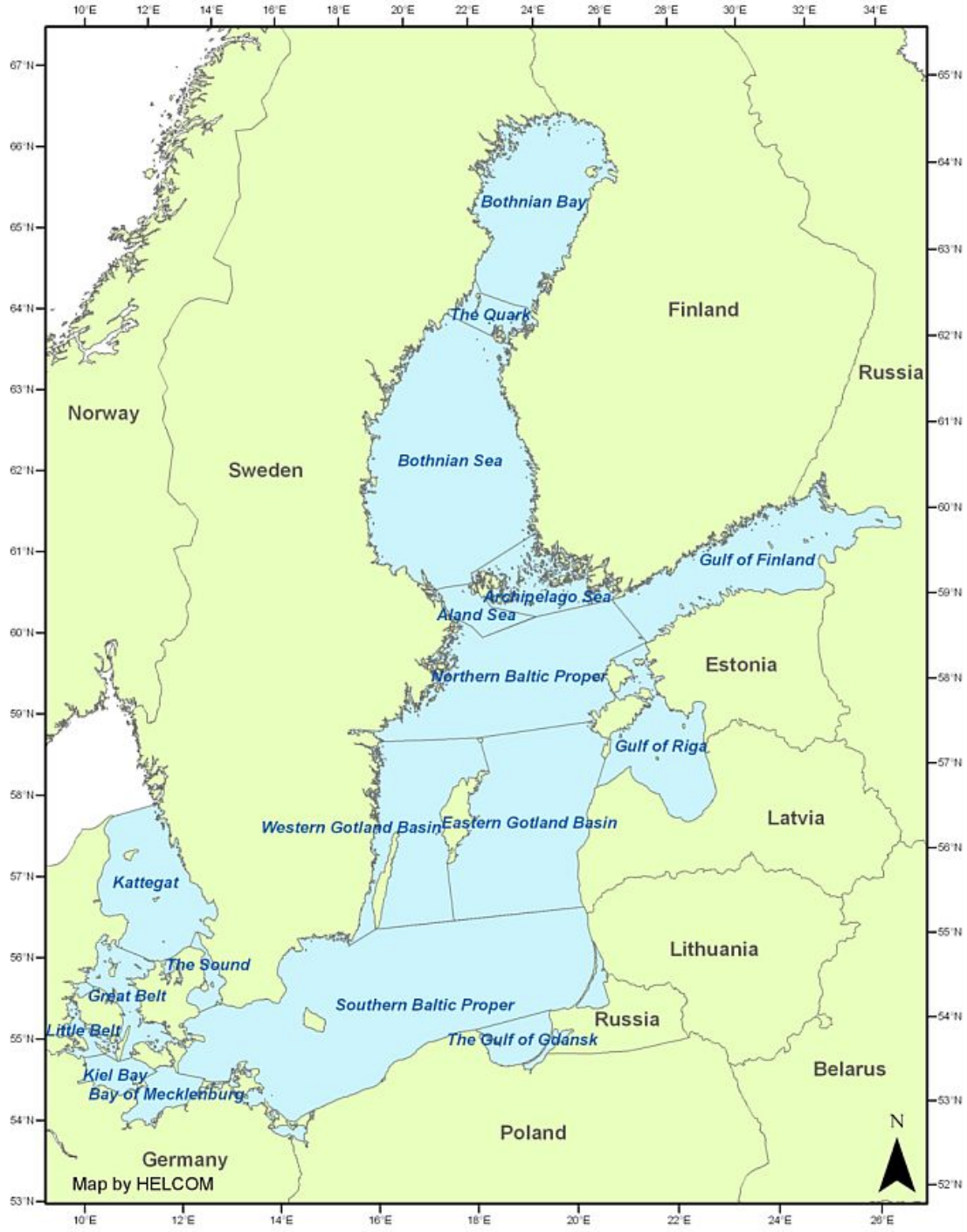

Fig. A1. Subdivision of the Baltic Sea. The basins mostly have specific water exchange characteristics. The map was downloaded from the Helcom website (HELCOM, 2010).[2]

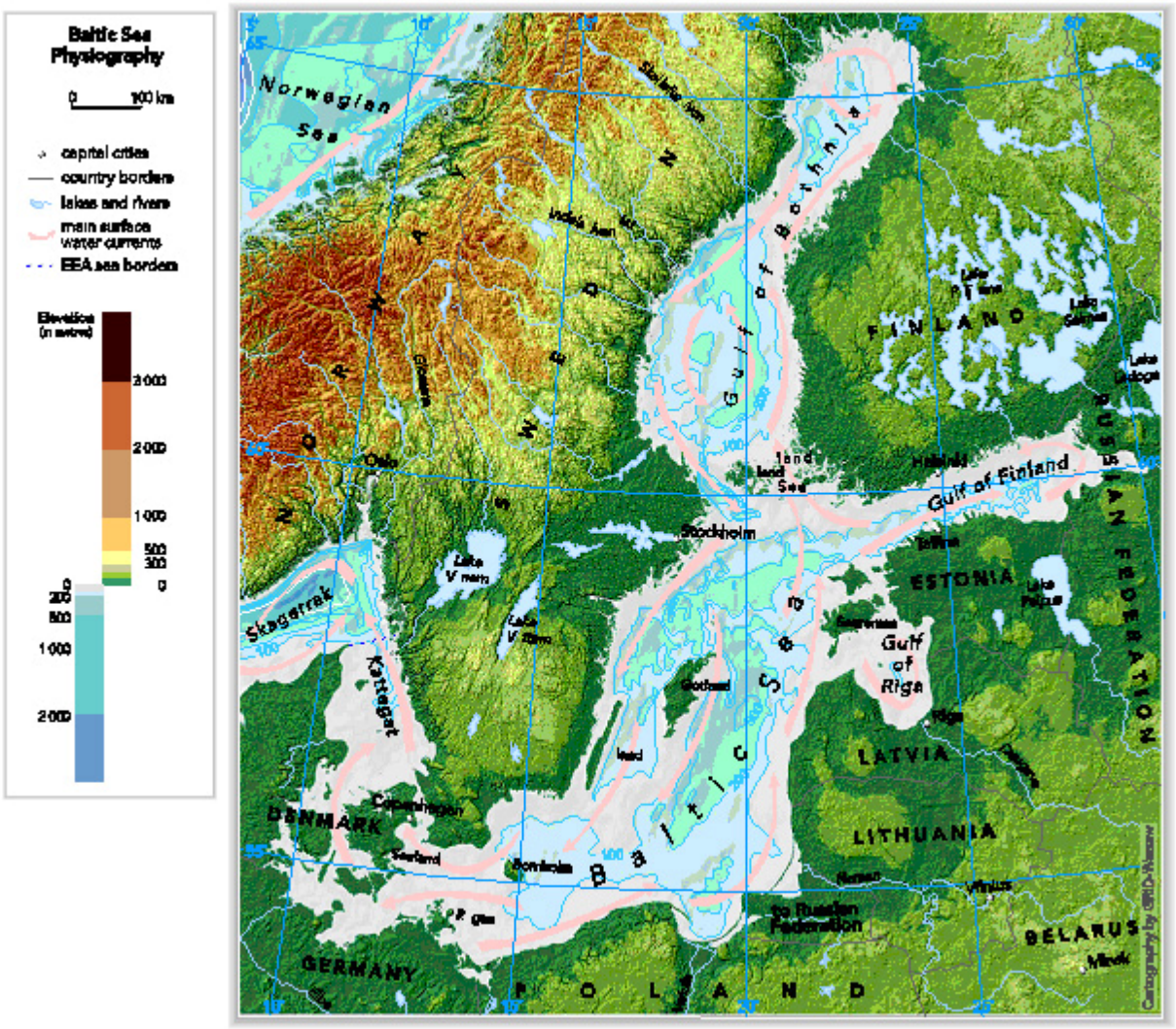

Fig. A2. Main currents in the Baltic Sea. The map was downloaded from the website of the European Environment Agency[1] (EEA, 2007).

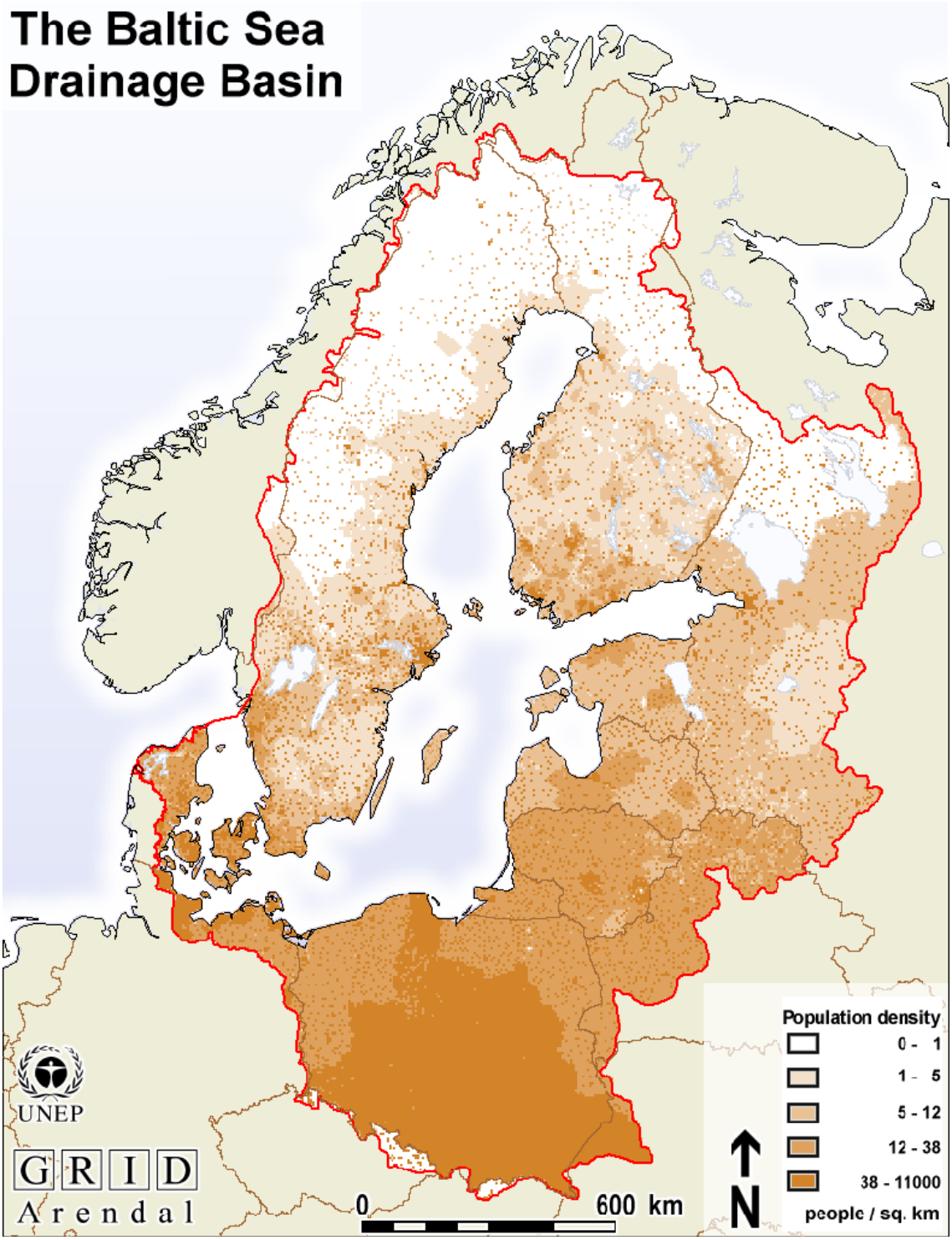

Fig. A3. Population density in the catchment of the Baltic Sea (UNEP/GRID-Arendal, 2001).[3]

Sample information

Table A1. Sample information

Sample ID	Sample name	Date	Time (hour)	Latitude	Longitude	Salinity (psu)	Temperature (°C)
1	Alkor320-AB 1	1 June 2008	0001	54.6167	12.2833	10.3	13.2
2	Alkor320-AB 2	1 June 2008	0250	54.7333	12.7917	10.3	12.6
3	Alkor320-AB 3	1 June 2008	0422	54.8917	13.0833	10.3	12.3
4	Alkor320-AB 4	1 June 2008	0550	54.9417	13.5000	10.2	12.4
5	Alkor320-AB 5	1 June 2008	0710	55.0167	14.0333	10.3	12.4
6	Alkor320-AB 6	1 June 2008	0849	55.1750	14.4167	10.3	12.4
7	Alkor320-AB 7	1 June 2008	1037	55.3333	14.6583	7.6	12.5
8	Alkor320-BB 3	1 June 2008	1500	55.6250	15.0000	7.3	12.9
9	Alkor320-BB 5	1 June 2008	1800	55.6250	15.5000	7.2	13.3
10	Alkor320-BB 7	1 June 2008	2125	55.6250	16.0000	7.3	13.3
11	Alkor320-BB 8	1 June 2008	2250	55.7917	16.0000	7.2	13.4
12	Alkor320-BB 11	2 June 2008	0310	55.7917	16.5000	7.1	13.6
13	Alkor320-BB 12	2 June 2008	0425	55.6250	16.5000	7.2	13.5
14	Alkor320-BB 20	2 June 2008	1430	55.2917	15.0000	7.3	14.0
15	Alkor320-BB 24	2 June 2008	2300	55.2917	16.0000	7.2	14.8
16	Alkor320-BB 26	3 June 2008	0140	55.2917	16.5000	7.2	14.7
17	Alkor320-SF 54	3 June 2008	0440	55.3483	17.0817	7.0	14.9
18	Alkor320-SF 47	3 June 2008	0843	55.2500	17.0833	6.7	13.7
19	Alkor320-BB 27	3 June 2008	1200	55.1250	16.5000	7.1	13.1
20	Alkor320-BB 31	3 June 2008	1750	55.1250	15.5000	7.2	13.0
21	Alkor320-BB 42	3 June 2008	2200	54.7917	15.0000	7.3	12.5
22	Alkor320-BB 44	4 June 2008	0400	54.6250	15.5000	7.2	12.3
23	Alkor320-BB 34	4 June 2008	0550	54.9583	15.2500	7.2	12.8
24	Alkor320-BB 38	4 June 2008	1305	54.7917	16.0000	7.2	13.0
25	Alkor320-BB 36	4 June 2008	1620	54.9583	16.0000	7.2	13.4
26	MSM08/3-1	18 June 2008	1230	54.3869	12.1045	17.3	26.6
27	MSM08/3-2	18 June 2008	2310	54.9256	13.5009	16.7	7.8
28	MSM08/3-3	19 June 2008	1230	55.2508	15.9821	16.5	7.5
29	MSM08/3-4	21 June 2008	1430	55.5165	15.5060	15.9	7.7
30	MSM08/3-5	22 June 2008	0915	54.9954	18.8568	16.3	7.3
31	MSM08/3-6	22 June 2008	1600	54.8665	19.2835	16.1	7.2
32	MSM08/3-7	23 June 2008	0700	55.9629	18.8823	15.3	7.4
33	MSM08/3-8	24 June 2008	1640	57.3062	20.0786	13.7	7.2
34	MSM08/3-9	27 June 2008	2230	58.2892	20.3412	15.6	6.2
35	MSM08/3-10	28 June 2008	0855	59.7511	19.7839	13.6	5.7
36	MSM08/3-11	28 June 2008	1400	60.1932	19.1182	14.1	5.0
37	MSM08/3-12	29 June 2008	1130	62.8018	20.2876	13.5	4.5
38	MSM08/3-13	30 June 2008	1855	64.7085	22.0538	14.1	2.8
39	MSM08/3-14	1 July 2008	0900	64.2510	21.7910	14.9	3.0
40	MSM08/3-15	1 July 2008	1410	63.5718	21.0615	15.0	3.2
41	MSM08/3-16	1 July 2008	2200	62.6309	19.2909	14.6	5.0
42	MSM08/3-17	2 July 2008	1325	62.5868	19.9688	15.0	4.8
43	MSM08/3-18	3 July 2008	0245	60.7170	19.1514	14.7	5.3
44	MSM08/3-19	3 July 2008	0510	60.2646	19.0133	14.8	5.2
45	MSM08/3-20	3 July 2008	1130	59.6190	20.8184	16.0	5.8
46	MSM08/3-21	3 July 2008	1235	59.4996	21.0005	16.6	5.9
47	MSM08/3-22	3 July 2008	1555	59.4998	21.9656	16.2	5.9
48	MSM08/3-23	4 July 2008	0750	59.7733	24.6789	16.5	5.5
49	MSM08/3-24	4 July 2008	0840	59.7979	24.7792	15.8	5.6

Sample ID	Sample name	Date	Time (hour)	Latitude	Longitude	Salinity (psu)	Temperature (°C)
50	MSM08/3-25	4 July 2008	1140	59.8316	25.9034	16.1	5.0
51	MSM08/3-26	4 July 2008	1415	59.7828	26.5841	17.9	4.4
52	MSM08/3-27	7 July 2008	0855	59.3690	23.5622	17.4	5.7
53	MSM08/3-28	7 July 2008	1435	59.1663	21.3168	17.3	6.4
54	MSM08/3-29	7 July 2008	1735	59.2311	20.3015	16.9	6.1
55	MSM08/3-30	7 July 2008	2030	59.2355	19.4088	15.7	5.8
56	MSM08/3-31	7 July 2008	2250	58.8600	19.0964	16.0	6.3
57	MSM08/3-32	8 July 2008	2135	58.5834	18.2327	16.1	6.9
58	MSM08/3-33	10 July 2008	0300	57.8661	17.6880	17.1	6.7
59	MSM08/3-34	10 July 2008	0730	57.2234	17.5814	17.5	7.2
60	MSM08/3-35	10 July 2008	0920	56.8789	17.4114	18.4	7.1
61	MSM08/3-36	10 July 2008	1210	56.4507	17.0694	17.0	7.3
62	MSM08/3-37	10 July 2008	1500	56.2859	17.6490	17.1	7.4
63	MSM08/3-38	11 July 2008	1030	55.7725	15.9269	17.2	7.6
64	MSM08/3-39	11 July 2008	2025	54.8434	12.9342	18.3	8.1
65	MSM08/3-40	12 July 2008	0505	55.1639	11.0584	18.9	13.0
66	MSM08/3-41	12 July 2008	0750	55.5967	10.8151	18.7	15.2
67	MSM08/3-42	12 July 2008	1055	56.0572	11.1000	18.8	17.2
68	MSM08/3-43	12 July 2008	1350	56.3485	11.6952	19.5	19.4
69	MSM08/3-44	12 July 2008	1735	56.4840	11.7218	19.3	19.3
70	MSM08/3-45	12 July 2008	2015	56.6921	11.0723	17.9	20.4
71	MSM08/3-46	13 July 2008	0115	57.1509	11.6894	18.0	21.3
72	MSM08/3-47	13 July 2008	0915	57.1916	11.6672	17.8	23.0
73	MSM08/3-48	13 July 2008	1605	57.8452	10.9909	17.6	31.8
74	MSM08/3-49	14 July 2008	1045	58.1457	10.2751	17.6	30.7

Blanks

Table A2. Average concentrations (ng L^{-1}) observed in blank samples during the two sampling campaigns

	Alkor 320	MSM08/3
PFBS	0.15	n.d.
PFPS	n.d.	n.d.
PFHxS	0.01	0.02
PFHpS	n.d.	n.d.
PFOS	0.02	0.01
PFNS	n.d.	n.d.
PFDS	n.d.	n.d.
TH-PFOS	n.d.	0.76
PFHxSi	n.d.	n.d.
PFOSi	0.01	0.01
PFDSi	n.d.	n.d.
PFBA	n.d.	0.08
PFPA	0.01	0.01
PFHxA	0.01	0.01
PFHpA	n.d.	0.01
PFOA	0.07	0.13
PFNA	0.01	0.03
PFDA	0.02	0.02
PFUnDA	0.01	0.01
PFDoDA	0.01	0.04
PFTriDA	n.d.	0.00
PFTeDA	n.d.	0.02
PFPeDA	n.d.	n.d.
PFHxDA	n.d.	0.01
PFHpDA	n.d.	n.d.
PFOcDA	n.d.	0.01
Me2PFOA	n.d.	n.d.
FOSA	0.08	0.12
NMeFOSA	n.d.	n.d.
NEtFOSA	n.d.	n.d.
NMeFOSE	n.d.	0.09
NEtFOSE	n.d.	n.d.
MeFBSA	n.d.	0.17
MeFBSE	0.12	0.10
FHEA (6:2 FTCA)	n.d.	n.d.
FOEA (8:2 FTCA)	n.d.	n.d.
FDEA (10:2 FTCA)	n.d.	n.d.
FHUEA (6:2 FTUCA)	n.d.	0.03
FOUEA (8:2 FTUCA)	0.05	n.d.
FDUEA (10:2 FTUCA)	n.d.	n.d.

Detection limits

Table A3. Average instrumental limits of detection (IDL, in pg, n=3) and method detection limits (MDL,in ng L-1, n=6) on the basis of signal to noise ratios of 3 (Ahrens et al. pers. comm.).

Analyte	IDL (pg)	MDL (ng L^{-1})	
		Dissolved phase	Particle phase
PFBS	0.191	0.352	0.174
PFHxS	0.220	0.140	0.045
PFHpS	0.199	0.029	n.d.
PFOS	0.264	0.061	0.022
PFDS	0.156	n.d.	n.d.
TH-PFOS	3.789	0.095	n.d.
PFHxSi	0.319	0.010	n.d.
PFOSi	0.221	0.028	0.006
PFDSi	0.307	n.d.	n.d.
PFBA	1.545	0.530	n.d.
PFPA	0.420	0.354	0.051
PFHxA	0.270	0.121	0.006
PFHpA	0.258	0.114	0.081
PFOA	0.278	0.075	0.03
PFNA	0.296	0.045	0.005
PFDA	0.444	0.047	0.087
PFUnDA	0.644	0.090	0.102
PFDoDA	0.381	0.026	0.228
PFTriDA	0.510	n.d.	n.d.
PFTeDA	0.752	n.d.	n.d.
PFHxDA	1.561	n.d.	n.d.
PFOcDA	1.160	n.d.	n.d.
Me2PFOA	0.801	0.011	n.d.
MeFBSA	3.263	n.d.	n.d.
PFOSA	0.941	0.021	0.017
MeFOSA	1.239	n.d.	n.d.
EtFOSA	1.205	n.d.	n.d.
MeFBSE	0.598	n.d.	n.d.
MeFOSE	0.803	n.d.	n.d.
EtFOSE	0.646	n.d.	0.014
FHEA	3.918	n.d.	n.d.
FOEA	2.520	n.d.	n.d.
FDEA	5.901	n.d.	n.d.
FHUEA	1.252	n.d.	n.d.
FOUEA	0.709	n.d.	n.d.
FDUEA	1.031	n.d.	n.d.

PFC concentrations

Table A4. Concentrations (ng L^{-1}) of PFC quantified in Baltic Sea surface water

<Blk, below the blank value; n.d., not detected; n.q.: not quantified

Sample ID	Sample name	PFBS	PFHxS	PFOS	PFBA	PFPA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFDoDA	FOSA
1	Alkor320-AB 1	<Blk	0.11	0.39	n.d.	0.11	0.29	0.12	0.78	0.26	0.15	0.13	n.d.
2	Alkor320-AB 2	0.07	0.18	0.23	n.d.	n.d.	0.19	0.16	0.38	0.23	n.d.	n.q.	n.d.
3	Alkor320-AB 3	<Blk	0.06	0.15	n.d.	0.07	0.22	0.12	0.44	0.18	0.06	n.q.	n.d.
4	Alkor320-AB 4	<Blk	0.05	0.20	n.d.	0.06	0.22	0.13	0.46	0.18	0.07	n.d.	n.d.
5	Alkor320-AB 5	<Blk	0.04	0.39	n.d.	n.d.	0.22	0.20	0.49	0.28	0.08	n.d.	n.d.
6	Alkor320-AB 6	0.01	0.08	0.31	0.17	0.09	0.18	0.09	0.38	0.19	0.05	n.q.	n.d.
7	Alkor320-AB 7	<Blk	0.16	0.25	n.d.	0.12	0.19	0.15	0.50	0.16	0.05	n.d.	n.d.
8	Alkor320-BB 3	0.16	0.19	0.24	n.d.	0.10	0.20	0.07	0.43	0.18	n.q.	n.d.	n.d.
9	Alkor320-BB 5	<Blk	0.07	0.29	n.d.	n.d.	0.18	0.13	0.34	0.16	n.q.	n.d.	n.d.
10	Alkor320-BB 7	<Blk	n.d.	0.24	n.d.	0.13	0.22	0.09	0.36	0.14	n.q.	n.d.	n.d.
11	Alkor320-BB 8	<Blk	0.03	0.25	n.d.	0.15	0.14	0.13	0.48	0.19	0.05	n.d.	n.d.
12	Alkor320-BB 11	<Blk	0.10	0.25	n.d.	0.11	0.21	0.16	0.38	0.18	n.q.	n.q.	0.06
13	Alkor320-BB 12	n.d.	0.05	0.17	n.d.	n.d.	0.21	0.12	0.37	0.12	n.q.	n.d.	n.d.
14	Alkor320-BB 20	n.d.	0.05	0.28	n.d.	0.05	0.16	0.11	0.37	0.13	0.05	n.d.	n.d.
15	Alkor320-BB 24	<Blk	0.01	0.21	n.d.	0.08	0.17	0.14	0.42	0.17	0.05	n.d.	n.d.
16	Alkor320-BB 26	<Blk	0.06	0.27	n.d.	0.07	0.22	0.12	0.36	0.17	0.05	n.d.	n.d.
17	Alkor320-SF 54	<Blk	0.14	0.11	n.d.	0.10	0.21	0.13	0.34	0.15	0.03	n.d.	n.d.
18	Alkor320-SF 47	<Blk	0.02	0.25	n.d.	0.16	0.19	0.13	0.39	0.16	0.05	n.d.	n.d.
19	Alkor320-BB 27	<Blk	0.05	0.18	n.d.	0.12	0.23	0.13	0.44	0.15	0.05	n.d.	n.d.
20	Alkor320-BB 31	0.01	n.d.	0.21	n.d.	0.07	0.17	0.16	0.45	0.19	n.d.	n.d.	n.d.
21	Alkor320-BB 42	<Blk	0.02	0.24	n.d.	0.09	0.16	0.15	0.37	0.16	n.q.	n.d.	n.d.
22	Alkor320-BB 44	n.d.	n.d.	0.04	n.d.	0.06	0.10	0.08	0.15	0.09	n.q.	n.d.	n.d.
23	Alkor320-BB 34	<Blk	0.08	0.20	n.d.	0.18	0.15	0.12	0.33	0.12	n.q.	n.d.	0.24
24	Alkor320-BB 38	0.01	0.03	0.14	n.d.	0.08	0.17	0.11	0.36	0.13	n.q.	n.d.	0.04
25	Alkor320-BB 36	<Blk	n.d.	0.19	n.d.	0.13	0.22	0.13	0.39	0.18	n.q.	n.d.	n.d.
26	MSM08/3-1	0.24	0.19	0.12	0.81	0.11	0.23	0.12	0.34	0.17	n.q.	n.d.	0.00
27	MSM08/3-2	0.14	0.17	0.15	0.59	0.09	0.13	0.13	0.37	0.28	n.q.	n.q.	0.03
28	MSM08/3-3	0.12	0.23	0.15	0.46	0.06	0.14	0.10	0.38	0.27	n.q.	0.05	0.08
29	MSM08/3-4	n.d.	0.11	0.18	1.33	0.13	0.15	0.13	0.40	0.23	<Blk	0.09	0.07
30	MSM08/3-5	n.d.	0.09	0.19	n.d.	0.04	0.12	0.10	0.42	0.23	n.q.	0.05	0.04
31	MSM08/3-6	0.16	0.15	0.18	1.12	0.10	0.15	0.12	0.41	0.24	n.q.	0.05	0.06
32	MSM08/3-7	0.13	0.21	0.15	n.d.	0.05	0.11	0.09	0.29	0.29	n.q.	0.05	0.07
33	MSM08/3-8	0.12	0.12	0.08	0.83	0.09	0.14	n.d.	0.40	0.34	n.q.	0.12	0.25
34	MSM08/3-9	0.19	0.04	0.12	n.d.	0.09	0.12	0.16	0.36	0.26	n.q.	0.06	0.16
35	MSM08/3-10	n.d.	0.06	0.16	0.64	0.09	0.13	0.08	0.26	0.30	n.q.	0.11	0.28
36	MSM08/3-11	n.d.	0.16	0.15	0.44	n.d.	0.12	0.09	0.33	0.31	n.q.	0.30	0.64
37	MSM08/3-12	n.d.	0.13	0.12	0.30	0.05	0.10	0.09	0.30	0.29	n.q.	0.06	0.23
38	MSM08/3-13	n.d.	0.11	0.12	0.59	0.10	0.09	0.09	0.12	0.33	n.q.	0.09	0.14
39	MSM08/3-14	0.26	0.12	0.05	0.89	n.d.	0.10	0.10	0.18	0.29	n.d.	0.06	0.17
40	MSM08/3-15	0.13	0.09	0.13	0.82	0.15	0.11	0.08	0.23	0.22	<Blk	n.d.	0.17
41	MSM08/3-16	n.d.	0.07	0.15	0.88	n.d.	0.12	0.09	0.25	0.25	n.q.	0.12	0.11
42	MSM08/3-17	0.12	n.d.	0.10	0.44	n.d.	0.14	0.09	0.29	0.21	n.d.	0.07	0.05
43	MSM08/3-18	0.18	0.03	0.14	0.88	0.07	0.12	0.07	0.24	0.28	n.q.	0.08	0.04
44	MSM08/3-19	0.14	0.07	0.11	0.99	0.08	0.11	0.08	0.28	0.29	n.q.	n.d.	0.01

Sample ID	Sample name	PFBS	PFHxS	PFOS	PFBA	PFPA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFDoDA	FOSA
45	MSM08/3-20	n.q.	0.07	0.06	n.d.	0.13	0.10	0.14	0.32	0.24	n.q.	0.08	0.08
46	MSM08/3-21	0.19	0.13	0.08	n.d.	n.d.	0.11	0.11	0.31	0.24	n.q.	0.10	0.05
47	MSM08/3-22	0.16	0.08	0.19	n.d.	n.d.	0.14	0.12	0.55	0.29	0.05	0.12	0.24
48	MSM08/3-23	0.11	0.08	0.24	0.57	n.d.	0.11	0.11	0.34	0.36	n.q.	0.08	0.08
49	MSM08/3-24	0.16	0.18	0.13	1.23	n.d.	0.16	0.16	0.42	0.42	0.07	n.d.	0.09
50	MSM08/3-25	0.26	0.03	0.13	1.07	0.10	0.14	0.12	0.34	0.28	n.q.	0.14	0.13
51	MSM08/3-26	0.36	0.04	0.24	1.00	0.04	0.14	0.18	0.45	0.50	0.05	n.d.	0.13
52	MSM08/3-27	n.d.	0.09	0.21	0.69	0.08	0.13	0.13	0.45	0.37	n.q.	0.13	0.11
53	MSM08/3-28	n.d.	0.13	0.16	n.d.	n.d.	0.13	0.11	0.35	0.49	n.q.	n.d.	0.13
54	MSM08/3-29	n.q.	0.10	0.18	0.73	0.04	0.15	0.09	0.36	0.30	n.d.	n.d.	0.04
55	MSM08/3-30	0.12	0.13	0.16	0.37	0.10	0.11	0.11	0.37	0.33	n.q.	0.14	0.03
56	MSM08/3-31	0.11	0.07	0.12	0.41	0.04	0.14	0.12	0.33	0.32	n.q.	n.d.	0.06
57	MSM08/3-32	n.d.	0.07	0.21	0.67	n.d.	0.15	0.11	0.43	0.33	n.d.	n.d.	0.15
58	MSM08/3-33	n.d.	0.10	0.14	1.78	n.d.	0.17	0.08	0.38	0.38	n.q.	n.d.	n.d.
59	MSM08/3-34	n.d.	0.12	0.10	0.75	n.d.	0.18	0.12	0.35	0.42	n.q.	n.d.	0.08
60	MSM08/3-35	n.d.	0.04	0.21	2.40	n.d.	0.16	0.12	0.56	0.85	0.08	n.d.	0.69
61	MSM08/3-36	n.d.	0.04	0.18	1.32	0.03	0.20	0.13	0.45	0.49	n.q.	n.d.	0.02
62	MSM08/3-37	n.d.	0.23	0.24	1.03	n.d.	0.12	0.11	0.37	0.47	0.08	n.d.	0.09
63	MSM08/3-38	0.24	n.d.	0.17	1.00	0.05	0.13	0.07	0.45	0.52	n.q.	n.d.	n.d.
64	MSM08/3-39	0.18	0.09	0.09	1.36	n.d.	0.18	0.10	0.48	0.45	n.q.	n.d.	n.d.
65	MSM08/3-40	0.40	0.11	0.10	0.59	0.08	0.21	0.11	0.70	0.47	0.08	n.d.	0.16
66	MSM08/3-41	0.48	0.16	0.20	0.59	0.08	0.20	0.10	0.72	0.58	0.08	n.d.	0.13
67	MSM08/3-42	0.43	0.08	0.27	0.44	0.07	0.19	0.14	0.57	0.39	n.q.	n.d.	n.d.
68	MSM08/3-43	0.76	0.08	0.21	1.72	0.12	0.17	0.10	0.53	0.38	0.05	n.d.	n.d.
69	MSM08/3-44	0.51	0.12	0.30	1.57	0.08	0.17	0.11	0.64	0.44	n.q.	n.d.	n.d.
70	MSM08/3-45	0.63	0.09	0.20	1.85	0.09	0.18	0.11	0.53	0.39	n.d.	0.16	0.13
71	MSM08/3-46	0.56	0.09	0.22	1.30	0.06	0.17	0.12	0.46	0.43	n.d.	0.14	n.d.
72	MSM08/3-47	0.68	0.07	0.20	1.70	0.06	0.16	0.08	0.58	0.43	n.q.	n.d.	n.d.
73	MSM08/3-48	0.73	0.10	0.19	1.16	0.06	0.18	0.12	0.73	0.53	n.q.	n.d.	n.d.
74	MSM08/3-49	0.51	0.05	0.12	1.46	0.07	0.13	0.12	0.51	0.29	n.q.	n.d.	n.d.

PFC composition

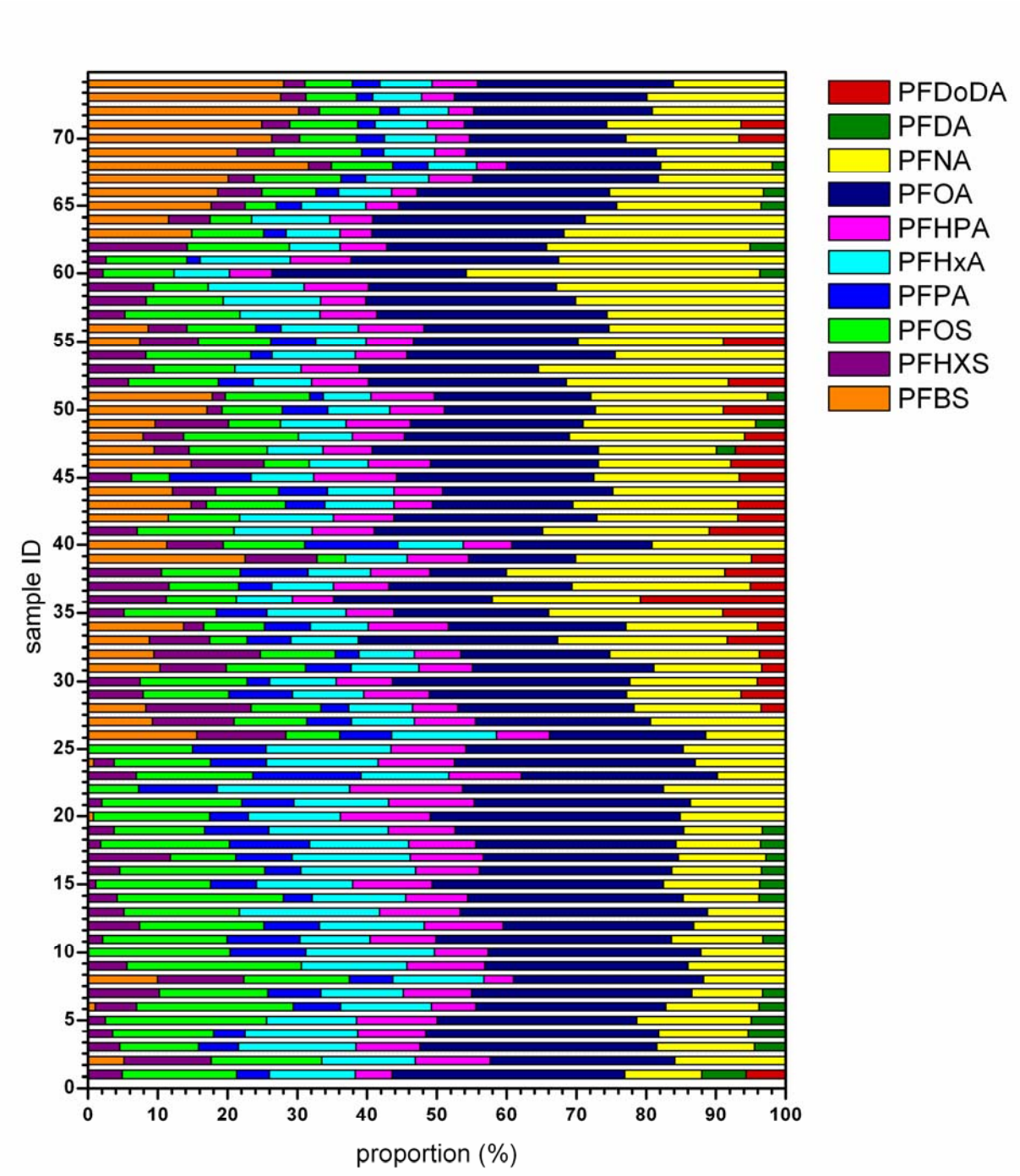

Fig. A4. PFC composition in Baltic Sea water samples. PFBA and FOSA were not included since absolute values of concentrations were uncertain. Note that there were blank Problems for PFBS in Alkor 320 samples (ID 1-25).

Spatial distribution

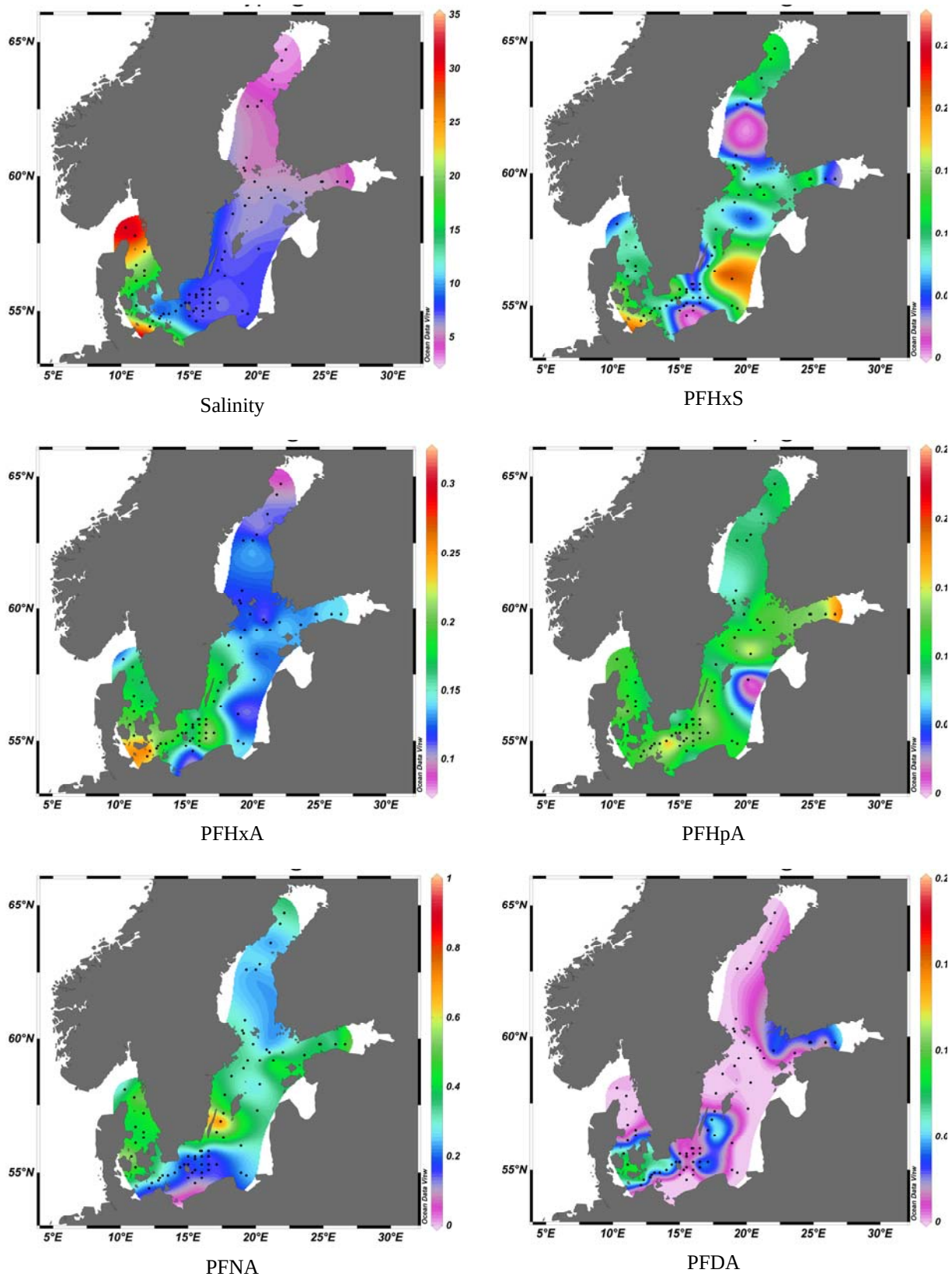

Fig. A5. Spatial distribution of salinity and various PFC in surface water of the Baltic Sea.

Information on analytes

Table A5. Analytes, acronyms, formula, supplier, purity, precursor and product ions for the MS/MS detection

Well. Lab., Wellington Laboratories; Lanc. Syn., Lancaster Synthesis. n.a., not available

Analyte	Abbreviation	Formula	Supplier (purity)	Precursor, product ion (*m*/*z*)
Perfluorobutane sulfonate	PFBS	$C_4F_9SO_2O^-$	Fluka (97%)	298.877, 79.8
Perfluoropentane sulfonate	PFPS	$C_5F_{11}SO_2O^-$	n.a.	348.939, 79.8
Perfluorohexane sulfonate	PFHxS	$C_6F_{13}SO_2O^-$	Fluka (98%)	398.894, 79.8
Perfluoroheptane sulfonate	PFHpS	$C_7F_{15}SO_2O^-$	Well. Lab. (>98%)	449.034, 79.3
Perfluorooctane sulfonate	PFOS	$C_8F_{17}SO_2O^-$	Well. Lab. (>98%)	498.971, 79.7
Perfluorononane sulfonate	PFNS	$C_9F_{19}SO_2O^-$	n.a.	548.926, 79.8
Perfluorodecane sulfonate	PFDS	$C_{10}F_{21}SO_2O^-$	Well. Lab. (>98%)	598.896, 79.5
6:2 fluorotelomer sulfonate	6:2 FTS	$C_6F_{13}C_2H_4SO_3^-$	ABCR (98%)	426.925, 406.7
Perfluoro-1-hexane sulfinate	PFHxSi	$C_6F_{13}SO_2^-$	Well. Lab. (>98%)	382.865, 319.0
Perfluoro-1-octane sulfinate	PFOSi	$C_8F_{17}SO_2^-$	Well. Lab. (>98%)	482.824, 418.9
Perfluoro-1-decane sulfinate	PFDSi	$C_{10}F_{21}SO_2^-$	Well. Lab. (>98%)	582.934, 518.9
Perfluorobutanoic acid	PFBA	C_3F_7COOH	ABCR (99%)	112.900, 168.7
Perfluoropentanoic acid	PFPA	C_4F_9COOH	Alfa Aesar (98%)	262.825, 218.9
Perfluorohexanoic acid	PFHxA	$C_5F_{11}COOH$	Fluka (97%)	312.934, 268.8
Perfluoroheptanoic acid	PFHpA	$C_6F_{13}COOH$	Lanc. Syn. (98%)	362.950, 318.9
Perfluorooctanoic acid	PFOA	$C_7F_{15}COOH$	Lanc. Syn. (95%)	412.987, 368.9
Perfluorononanoic acid	PFNA	$C_8F_{17}COOH$	Lanc. Syn. (97%)	462.908, 418.9
Perfluorodecanoic acid	PFDA	$C_9F_{19}COOH$	Lanc. Syn. (97%)	512.876, 469.0
Perfluoroundecanoic acid	PFUnDA	$C_{10}F_{21}COOH$	ABCR (96%)	562.865, 519.0
Perfluorododecanoic acid	PFDoDA	$C_{11}F_{23}COOH$	Alfa Aesar (96%)	612.991, 568.9
Perfluorotridecanoic acid	PFTriDA	$C_{12}F_{25}COOH$	Well. Lab. (>98%)	663.094, 618.9
Perfluorotetradecanoic acid	PFTeDA	$C_{13}F_{27}COOH$	Alfa Aesar (96%)	713.036, 669.0
Perfluorotridecanoic acid	PFPDA	$C_{14}F_{29}COOH$	n.a.	762.980, 718.9
Perfluorohexadecanoic acid	PFHxDA	$C_{15}F_{31}COOH$	Alfa Aesar (95%)	812.840, 769.1
Perfluoroheptadecanoic acid	PFHpDA	$C_{16}F_{33}COOH$	n.a.	862.980, 818.9
Perfluorooctadecanoic acid	PFOcDA	$C_{17}F_{35}COOH$	Alfa Aesar (97%)	912.870, 869.0
3,7-dimethylperfluorooctanoic acid	Me_2PFOA	$C_9F_{19}COOH$	Alfa Aesar (97%)	512.885, 468.9
N-methylperfluorobutane sulfonamide	MeFBSA	$C_4F_9SO_2NH(CH_3)$	3M (n.a.)	311.914, 218.8
Perfluorooctane sulfonamide	FOSA	$C_8F_{17}SO_2NH_2$	ABCR (97%)	497.896, 77.9

Analyte	Abbreviation	Formula	Supplier (purity)	Precursor, product ion (*m*/*z*)
N-methyl perfluorooctane sulfonamide	MeFOSA	$C_8F_{17}SO_2NH(CH_3)$	3M (n.a.)	511.849, 168.9
N-ethyl perfluorooctane sulfonamide	EtFOSA	$C_8F_{17}SO_2NH(C_2H_5)$	ABCR (95%)	526.008, 169.0
N-methylperfluorobutane sulfonamidoethanol	MeFBSE	$C_4F_9SO_2N(CH_3)C_2H_4OH$	3M (n.a.)	416.047, 59.0
N-methyl perfluorooctane sulfonamidoethanol	MeFOSE	$C_8F_{17}SO_2N(CH_3)C_2H_4OH$	3M (n.a.)	616.004, 58.9
N-ethyl perflurooctane sulfonamidoethanol	EtFOSE	$C_8F_{17}SO_2N(C_2H_5)C_2H_4OH$	3M (n.a.)	630.109, 58.8
2-Perfluorohexyl ethanoic acid	FHEA	$C_6F_{13}CH_2COOH$	Well. Lab. (>98%)	376.945, 292.8
2-Perfluorooctyl ethanoic acid	FOEA	$C_8F_{17}CH_2COOH$	Well. Lab. (>98%)	476.909, 392.9
2-Perfluorodecyl ethanoic acid	FDEA	$C_{10}F_{21}CH_2COOH$	Well. Lab. (>98%)	577.011, 493.0
2H-Perfluoro-2-octenoic acid	FHUEA	$C_6F_{12}CHCOOH$	Well. Lab. (>98%)	356.885, 293.0
2H-Perfluoro-2-decenoic acid	FOUEA	$C_8F_{16}CHCOOH$	Well. Lab. (>98%)	456.803, 292.8
2H-Perfluoro-2-dodecenoic acid	FDUEA	$C_{10}F_{20}CHCOOH$	Well. Lab. (>98%)	556.937, 493.1
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	$C_4F_9[1,2,3,4\text{-}^{13}C_4]F_8SO_2O^-$	Well. Lab. (>98%)	502.899, 79.5
Perfluoro-1-[1,2,3,4-$^{13}C_4$]octanesulfinate	[$^{13}C_4$]-PFOSi	$C_4F_9[1,2,3,4\text{-}^{13}C_4]F_8SO_2^-$	Well. Lab. (>90%)	486.859, 422.9
Perfluoro-n-(1,2,3,4-$^{13}C_4$)butanoic acid	[$^{13}C_4$]-PFBA	$2,3,4\text{-}^{13}C_3F_7{}^{13}COOH$	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	$C_4F_9[2,3,4,5\text{-}^{3}C_4]F_8{}^{13}COOH$	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-$^{13}C_2$]dodecanoic acid	[$^{13}C_2$]-PFDoDA	$C_{10}F_{21}{}^{13}CF_2{}^{13}COOH$	Well. Lab. (>98%)	614.913, 569.9
N-methyl-d_3-perfluoro-1-octanesulfonamide	d_3-N-MeFOSA	$C_9D_3HF_{17}NO_2S$	Well. Lab. (>98%)	514.920, 168.8
N-ethyl-d_5-perfluoro-1-octanesulfonamide	d_5-N-EtFOSA	$C_{10}D_5HF_{17}NO_2S$	Well. Lab. (>98%)	530.984, 168.8
2-(N-deuteriomethylperfluoro-1-octanesulfoneamido)-1,1,2,2-tetradeuterioethanol	d_7-N-MeFOSE	$C_8F_{17}SO_2N(CD_3)C_2D_4OH$	Well. Lab. (>98%)	623.058, 58.9
2-(N-deuterioethylperfluoro-1-octanesulfoneamido)-1,1,2,2-tetradeuterioethanol	d_9-N-EtFOSE	$C_8F_{17}SO_2N(C_2D_5)C_2D_4OH$	Well. Lab. (>98%)	639.054, 58.9
2-Perfluorohexyl-[1,2-$^{13}C_2$]ethanoic acid	[$^{13}C_2$]-FHEA	$C_6F_{13}{}^{13}CH_2{}^{13}COOH$	Well. Lab. (>98%)	378.912, 294.0
2-Perfluorooctyl-[1,2-$^{13}C_2$]ethanoic acid	[$^{13}C_2$]-FOEA	$C_8F_{17}{}^{13}CH_2{}^{13}COOH$	Well. Lab. (>98%)	478.911, 393.8
2-Perfluorodecyl-[1,2-$^{13}C_2$]ethanoic acid	[$^{13}C_2$]-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-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	d_5-EtFOSAA	$C_8F_{17}SO_2N(C_2D_2\ C_2D_3)C_2H_2CO_2H$	Well. Lab. (>98%)	589.015, 418.7

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