

Accessory publication**Perfluorinated compounds in red-throated divers from the German Baltic Sea: new findings from their distribution in 10 different tissues**

Janne Rubarth,^{A,B,E} Annetrin Dreyer,^{A,C} Nils Guse,^D Jürgen W. Einax^B and Ralf Ebinghaus^A

^AHelmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht, Germany.

^BFriedrich Schiller University of Jena, Lessingstraße 8, D-07743 Jena, Germany.

^CEurofins GfA GmbH, Air Monitoring, Stenzelring 14b, D-21107 Hamburg, Germany.

^DResearch and Technology Centre Westcoast (FTZ), University of Kiel, Hafentörn 1, D-25761 Büsum, Germany.

^ECorresponding author. Present address: Leibniz Institute for Baltic Sea Research Warnemünde, Seestraße 15, D-18119 Rostock, Germany. Email: janne.rubarth@io-warnemuende.de

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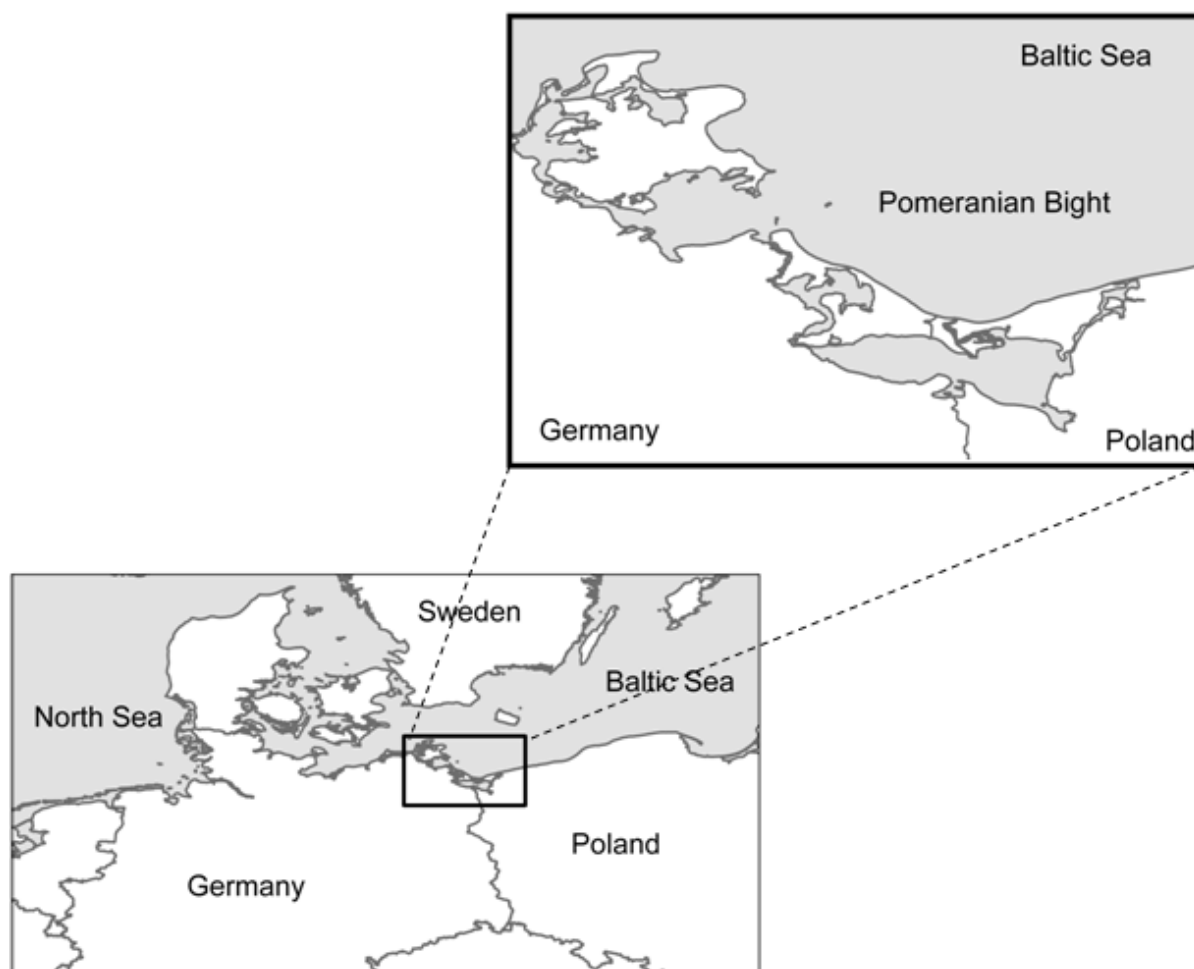


Fig. A1. Map of the Southern Baltic Sea with close-up of the Pomeranian Bight (study area).

Analytical standards and chemicals

Table A1. Analytical standards, their acronyms, producers and purities

Well. Lab, Wellington Laboratories; Lanc. Syn, Lancaster Synthesis

Compound	Abbreviation	Producer (purity (%))
Potassium perfluoro- <i>n</i> -butane sulfonate	PFBS	Fluka (97 %)
Sodium perfluoro- <i>n</i> -hexane sulfonate	PFHxS	Fluka (98 %)
Sodium perfluoro- <i>n</i> -heptane sulfonate	PFHpS	Well. Lab (> 98 %)
Sodium perfluoro- <i>n</i> -octane sulfonate	PFOS	Well. Lab (> 98 %)
Sodium perfluoro- <i>n</i> -decane sulfonate	PFDS	Well. Lab (> 98 %)
Perfluoro- <i>n</i> -heptanoate	PFHpA	Lanc. Syn (98 %)
Perfluoro- <i>n</i> -octanoate	PFOA	Lanc. Syn (95 %)
Perfluoro- <i>n</i> -nonanoate	PFNA	Lanc. Syn (97 %)
Perfluoro- <i>n</i> -decanoate	PFDA	Lanc. Syn (97 %)
Perfluoro- <i>n</i> -undecanoate	PFUnDA	ABCR (96 %)
Perfluoro- <i>n</i> -dodecanoate	PFDoDA	Alfa Aesar (96 %)
Perfluoro- <i>n</i> -tridecanoate	PFTriDA	Well. Lab (> 98 %)
Perfluoro- <i>n</i> -tetradecanoate	PFTeDA	Alfa Aesar (96 %)
Perfluoro- <i>n</i> -hexadecanoate	PFHxDA	Alfa Aesar (95 %)
Perfluoro- <i>n</i> -octadecanoate	PFOcDA	Alfa Aesar (97 %)
Perfluoro-1-octane sulfonamide	PFOSA	ABCR (97 %)
<i>N</i> -methyl perfluoro-1-octane sulfonamide	<i>N</i> -MeFOSA	Well. Lab (> 98 %)
<i>N</i> -ethyl perfluoro-1-octane sulfonamide	<i>N</i> -EtFOSA	Well. Lab (> 98 %)
2-(<i>N</i> -methyl perfluoro-1-octane sulfonamido)-ethanol	<i>N</i> -MeFOSE	Well. Lab (> 98 %)
2-(<i>N</i> -ethylperfluoro-1-octane sulfonamido)-ethanol	<i>N</i> -EtFOSE	Well. Lab (> 98 %)
Sodium perfluoro-1-hexane [¹⁸ O ₂]-sulfonate	[¹⁸ O ₂]-PFHxS	Well. Lab (> 98 %)
Sodium perfluoro-1-[1,2,3,4- ¹³ C ₄]-octane sulfonate	[¹³ C ₄]-PFOS	Well. Lab (> 98 %)
Perfluoro- <i>n</i> -[1,2,3,4- ¹³ C ₄]-octanoate	[¹³ C ₄]-PFOA	Well. Lab (> 98 %)
Perfluoro- <i>n</i> -[1,2,3,4,5- ¹³ C ₅]-nonanoate	[¹³ C ₅]-PFNA	Well. Lab (> 98 %)
Perfluoro- <i>n</i> -[1,2- ¹³ C ₂]-decanoate	[¹³ C ₂]-PFDA	Well. Lab (> 98 %)
Perfluoro- <i>n</i> -[1,2- ¹³ C ₂]-undecanoate	[¹³ C ₂]-PFUnDA	Well. Lab (> 98 %)
Perfluoro- <i>n</i> -[1,2- ¹³ C ₂]-dodecanoate	[¹³ C ₂]-PFDoDA	Well. Lab (> 98 %)
Perfluoro-1-[¹³ C ₈]-octane sulfonamide	[¹³ C ₈]-PFOSA	Well. Lab (> 98 %)
<i>N</i> -methyl d ₃ -perfluoro-1-octane sulfonamide	d ₃ - <i>N</i> -MeFOSA	Well. Lab (> 98 %)
<i>N</i> -ethyl d ₅ -perfluoro-1-octane sulfonamide	d ₅ - <i>N</i> -EtFOSA	Well. Lab (> 98 %)
2-(<i>N</i> -deuteriomethyl perfluoro-1-octane sulfonamido)-1,1,2,2-tetradeuterioethanol	d ₇ - <i>N</i> -MeFOSE	Well. Lab (> 98 %)
2-(<i>N</i> -deuterioethyl perfluoro-1-octane sulfonamido)-1,1,2,2-tetradeuterioethanol	d ₉ - <i>N</i> -EtFOSE	Well. Lab (> 98 %)

Table A2. Chemicals used for samples' preparation, their purities and producers

Chemical	Purity (%)	Producer
methanol Picograde	≥ 99.0	Merck
acetonitrile LiChrosolv	≥ 99.9	Merck
glacial acetic acid	100	Merck
ammonium acetate Fractopur	≥ 98.0	Merck

Dissection reports

Table A3. Dissection reports of four red-throated divers collected near Usedom, Mecklenburg – West Pomerania, Germany in March and April 2005

Dissection took place in November 2009 at the Research and Technology Centre Westcoast, Büsum, Germany (FTZ)

Red-throated divers (<i>Gavia stellata</i>)				
Age	<1	<1	<1	<1
Date of finding	17 March 2005	17 March 2005	4 April 2005	22 March 2005
Locality	Ahlbeck, Germany	Ahlbeck, Germany	Ahlbeck, Germany	Ahlbeck, Germany
Cause of death	By-catch in set net fisheries	By-catch in set net fisheries	By-catch in set net fisheries	By-catch in set net fisheries
Comments	Right wing is missing	Right wing is missing	None	None
Head length (mm)	132	123	119	118
Tarsus length (mm)	74	70	70	72
Wing length (mm)	292	261	225	266
Tissue weight (g)				
Blood ^{[1],A}	120	120	120	120
Brain ^B	4.9	5.5	4.0	4.4
Fatty tissue ^{[2],A}	500	500	500	500
Gall bladder ^{C,B}	1.7	1.8	1.1	1.3
Heart ^A	22	19	17	19
Kidney ^{D,A}	42	52	26	40
Liver ^A	67	70	60	61
Lung ^A	33	31	24	25
Muscle tissue ^{[2],A}	500	500	500	500
Spleen ^B	1.3	1.5	1.0	1.3
Σtissue weight	1292	1301	1253	1272
Body weight ^[3]	1500	1500	1500	1500

^APartially sampled.

^BCompletely sampled.

^CWithout bile.

^DWeight of left and right kidney.

Standard solution**Table A4. Compounds and concentrations of native analytical standards in standard solution 1**

Compound	$C_{\text{standard solution 1}}$ ($\mu\text{g L}^{-1}$)
PFBS	4
PFHxS	20
PFHpS	4
PFOS	100
PFDS	4
PFHpA	4
PFOA	4
PFNA	20
PFDA	4
PFUnDA	20
PFDoDA	20
PFTriDA	20
PFTeDA	4
PFHxDA	4
PFOcDA	4
PFOSA	60
<i>N</i> -MeFOSA	4
<i>N</i> -EtFOSA	4
<i>N</i> -MeFOSE	4
<i>N</i> -EtFOSE	4

Precursor and product ion**Table A5. Compounds, their precursor and product ion as well as their retention times during HPLC analysis**

Compound	Precursor ion (<i>m/z</i>)	Product ion (<i>m/z</i>)	Retention time (min)
PFBS	298.9	79.8	10.3
PFHxS	398.9	79.8	12.9
PFHpS	449.0	79.3	14.6
PFOS	499.0	79.6	16.7
PFDS	598.9	79.5	21.7
PFHpA	363.0	318.8	12.9
PFOA	413.0	369.0	14.7
PFNA	462.9	418.9	16.9
PFDA	512.9	469.0	19.3
PFUnDA	562.9	519.0	22.0
PFDoDA	613.0	568.9	24.6
PFTriDA	663.1	618.9	27.2
PFTeDA	713.0	669.0	29.6
PFHxDA	812.8	769.1	33.6
PFOcDA	912.9	869.0	36.0
PFOSA	497.9	77.9	21.5
<i>N</i> -MeFOSA	511.8	168.9	25.5
<i>N</i> -EtFOSA	526.0	169.0	26.7
<i>N</i> -MeFOSE	616.0	58.9	25.5
<i>N</i> -EtFOSE	630.1	58.8	27.4
[¹⁸ O ₂]-PFHxS	403.0	83.9	12.8
[¹³ C ₄]-PFOS	502.9	79.5	16.7
[¹³ C ₄]-PFOA	417.0	371.8	14.7
[¹³ C ₅]-PFNA	467.9	423.0	16.9
[¹³ C ₂]-PFDA	514.9	469.8	19.3
[¹³ C ₂]-PFUnDA	565.0	519.8	22.0
[¹³ C ₂]-PFDoDA	614.9	569.9	24.6
[¹³ C ₈]-PFOSA	506.1	77.8	20.6
d ₃ - <i>N</i> -MeFOSA	514.9	168.8	25.0
d ₅ - <i>N</i> -EtFOSA	531.0	168.8	27.3
d ₇ - <i>N</i> -MeFOSE	623.1	58.9	25.5
d ₉ - <i>N</i> -EtFOSE	639.1	58.9	27.3

Recovery rates of mass-labelled compounds for investigated samples

Table A6. Recovery rates and absolute standard deviation of mass-labelled compounds for the investigated tissue samples ($n = 10$)

n.a., not analysed

Compound	Recovery rates (%) \pm absolute standard deviation (%)									
	Blood	Brain	Fatty tissue	Gall bladder	Heart	Kidney	Liver	Lung	Muscle	Spleen
[¹⁸ O ₂]-PFHxS	66 \pm 18	106 \pm 14	79 \pm 14	68 \pm 13	81 \pm 5	71 \pm 23	65 \pm 8	116 \pm 23	71 \pm 17	70 \pm 9
[¹³ C ₄]-PFOS	63 \pm 4	100 \pm 17	89 \pm 42	74 \pm 22	89 \pm 5	80 \pm 26	82 \pm 10	99 \pm 26	90 \pm 13	80 \pm 15
[¹³ C ₄]-PFOA	67 \pm 17	104 \pm 14	83 \pm 19	61 \pm 19	77 \pm 11	77 \pm 27	63 \pm 8	117 \pm 19	77 \pm 22	74 \pm 12
[¹³ C ₅]-PFNA	60 \pm 3	98 \pm 9	86 \pm 23	69 \pm 19	84 \pm 7	83 \pm 21	77 \pm 6	101 \pm 17	81 \pm 6	83 \pm 4
[¹³ C ₂]-PFDA	56 \pm 2	99 \pm 18	81 \pm 32	70 \pm 21	87 \pm 5	78 \pm 21	75 \pm 10	93 \pm 22	78 \pm 12	76 \pm 16
[¹³ C ₂]-PFUnDA	60 \pm 7	101 \pm 13	91 \pm 19	73 \pm 21	84 \pm 10	81 \pm 15	69 \pm 3	97 \pm 22	78 \pm 11	74 \pm 4
[¹³ C ₂]-PFDoDA	55 \pm 3	104 \pm 16	81 \pm 15	71 \pm 19	79 \pm 5	78 \pm 15	70 \pm 2	90 \pm 23	83 \pm 12	79 \pm 4
[¹³ C ₈]-PFOSA	52 \pm 5	100 \pm 21	82 \pm 26	76 \pm 18	86 \pm 6	72 \pm 23	76 \pm 11	89 \pm 30	82 \pm 12	75 \pm 6
d ₃ - <i>N</i> -MeFOSA	55 \pm 5	90 \pm 11	57 \pm 5	64 \pm 17	69 \pm 6	63 \pm 21	56 \pm 12	83 \pm 20	75 \pm 17	55 \pm 4
d ₅ - <i>N</i> -EtFOSA	56 \pm 6	94 \pm 21	n.a.	60 \pm 11	86 \pm 17	73 \pm 26	54 \pm 6	88 \pm 27	n.a.	66 \pm 28
d ₇ - <i>N</i> -MeFOSE	55 \pm 6	98 \pm 7	76 \pm 10	65 \pm 2	77 \pm 5	80 \pm 27	71 \pm 7	93 \pm 3	86 \pm 11	69 \pm 15
d ₉ - <i>N</i> -EtFOSE	54 \pm 7	95 \pm 17	n.a.	90 \pm 30	n.a.	82 \pm 13	66 \pm 17	90 \pm 19	n.a.	n.a.

Method detection and method quantification limits

Table A7. Method detection limits (ng g⁻¹) and method quantification limits (ng g⁻¹) of investigated perfluorinated compounds in the investigated tissue samples (*n* = 10)

The compounds which were not detected in any of the samples are not listed. n.d., not detected

Compound	Blood		Brain		Fatty tissue		Gall bladder		Heart		Kidney		Liver		Lung		Muscle		Spleen	
	MDL	QL	MDL	QL	MDL	QL	MDL	QL	MDL	QL	MDL	QL	MDL	QL	MDL	QL	MDL	QL	MDL	QL
PFHxS	0.081	0.242	0.049	0.146	0.094	0.283	0.449	1.35	0.148	0.445	0.109	0.325	0.162	0.487	0.123	0.369	0.176	0.528	0.171	0.512
PFHpS	0.028	0.082	0.043	0.129	0.095	0.284	0.165	0.496	0.037	0.111	0.520	1.560	0.403	1.21	0.040	0.121	0.062	0.185	0.108	0.324
PFOS	1.29	3.86	0.588	1.77	2.11	6.33	2.81	8.43	1.11	3.33	0.789	2.37	5.45	16.4	0.803	2.41	0.821	2.46	3.37	10.1
PFDS	0.060	0.179	0.054	0.162	0.076	0.227	0.078	0.233	0.057	0.170	0.091	0.273	0.126	0.378	0.054	0.161	0.029	0.086	0.103	0.309
PFHpA	0.014	0.041	0.054	0.161	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.361	1.08	0.023	0.069	n.d.	n.d.	n.d.	n.d.
PFOA	0.054	0.162	0.034	0.102	0.046	0.137	0.116	0.349	0.025	0.074	0.112	0.335	0.089	0.267	0.025	0.075	0.029	0.087	0.033	0.100
PFNA	0.128	0.383	0.116	0.349	0.277	0.831	0.391	1.17	0.133	0.400	0.227	0.682	0.199	0.596	0.210	0.631	0.107	0.319	0.286	0.859
PFDA	0.022	0.066	0.025	0.075	0.059	0.177	0.077	0.230	0.029	0.088	0.043	0.130	0.085	0.256	0.054	0.161	0.027	0.081	0.109	0.327
PFUnDA	0.143	0.429	0.180	0.540	0.136	0.407	0.552	1.66	0.160	0.480	0.256	0.768	0.199	0.596	0.128	0.383	0.190	0.571	0.363	1.089
PFDoDA	0.073	0.220	0.143	0.428	0.106	0.317	0.362	1.09	0.198	0.595	0.110	0.331	0.137	0.410	0.143	0.428	0.110	0.329	0.156	0.468
PFTriDA	0.101	0.304	0.335	1.01	0.167	0.501	0.236	0.709	0.064	0.191	0.085	0.255	0.163	0.489	0.178	0.534	0.094	0.281	0.195	0.584
PFTeDA	0.016	0.046	0.108	0.323	0.042	0.125	0.087	0.262	0.115	0.344	0.052	0.153	0.029	0.087	0.039	0.117	0.069	0.208	0.066	0.198
PFHxDA	n.d.	n.d.	0.027	0.081	n.d.	n.d.	n.d.	n.d.	0.060	0.178	0.061	0.183	0.028	0.085	0.034	0.101	n.d.	n.d.	0.058	0.175
PFOcDA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.021	0.062	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
PFOSA	0.230	0.689	0.728	2.19	2.13	6.39	1.26	3.79	0.495	1.49	0.514	1.54	1.45	4.35	0.366	1.10	1.06	3.19	2.10	6.31

PFC concentrations in investigated tissue samples

Table A8. PFC concentrations (ng g⁻¹ wet weight) of blood, brain, fatty tissue, gall bladder, heart, kidney, liver, lung, muscle and spleen in four red-throated divers

n.d., not detected; n.a., not analysed; <MQL, below the method quantification limits

Compound	Blood				Brain				Fatty tissue				Gall bladder				Heart				
	bird1	bird2	bird3	bird4	bird1	bird2	bird3	bird4	bird1	bird2	bird3	bird4	bird1	bird2	bird3	bird4	bird1	bird2	bird3	bird4	
PFBS	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	
PFHxS	8.15	3.34	3.28	2.73	1.52	0.64	1.02	0.72	<MQL	0.53	0.79	2.36	2.71	<MQL	3.78	2.50	2.60	2.23	1.93	1.61	
PFHpS	n.a.	n.a.	0.84	0.75	0.42	0.18	0.65	0.33	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	1.55	n.d.	0.61	0.74	1.14	0.52	
PFOS	59.3	n.a.	57.01	103.15	29.55	30.96	50.03	50.91	<MQL	12.86	53.26	97.02	55.20	45.98	149.34	87.50	96.94	64.64	74.74	52.51	
PFDS	0.23	<MQL	0.23	<MQL	0.64	0.38	0.62	0.47	n.d.	<MQL	<MQL	n.d.	n.d.	<MQL	0.29	<MQL	<MQL	<MQL	<MQL	<MQL	
PFHpA	0.08	n.d.	n.d.	n.d.	<MQL	n.d.	<MQL	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	
PFOA	n.a.	n.a.	0.64	1.32	0.53	0.19	0.55	0.26	0.149	0.16	0.33	0.41	n.d.	<MQL	1.00	0.36	0.66	0.85	0.72	0.69	
PFNA	1.85	3.02	1.55	1.68	1.13	0.48	1.05	0.55	<MQL	<MQL	1.35	<MQL	2.62	1.42	4.53	1.81	1.93	1.72	3.07	1.16	
PFDA	0.48	0.46	0.48	0.31	0.65	0.32	0.42	0.31	<MQL	<MQL	0.28	0.23	0.43	0.48	1.12	0.70	0.60	0.57	0.47	0.29	
PFUnDA	4.89	4.27	3.79	2.24	6.41	3.74	8.86	3.47	0.436	0.61	1.91	1.36	2.56	2.70	9.57	3.17	2.49	3.10	3.35	1.93	
PFDoDA	1.29	1.17	1.41	0.63	3.70	1.90	4.89	2.19	<MQL	<MQL	0.54	0.54	<MQL	<MQL	2.62	<MQL	0.86	1.02	1.42	0.82	
PFTriDA	2.09	2.00	1.93	1.17	11.02	6.62	11.99	4.86	<MQL	<MQL	0.72	0.82	<MQL	1.24	3.25	1.85	1.47	2.34	2.29	1.72	
PFTeDA	0.24	0.52	0.30	0.35	3.80	1.30	2.38	1.81	n.d.	n.d.	n.d.	n.d.	<MQL	0.43	0.64	0.47	n.d.	n.d.	n.d.	n.d.	
PFHxDA	n.d.	n.d.	n.d.	n.d.	<MQL	<MQL	<MQL	<MQL	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<MQL	<MQL	<MQL	<MQL
PFOcDA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	
PFOSA	12.28	14.71	12.53	46.60	23.04	6.54	8.39	11.66	<MQL	<MQL	11.07	16.00	12.14	10.66	19.92	24.50	21.09	10.32	8.70	14.73	
<i>N</i> -MeFOSA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	
<i>N</i> -EtFOSA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	
<i>N</i> -MeFOSE	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	

Table A8. (Cont.)

Compound	Blood				Brain				Fatty tissue				Gall bladder				Heart			
	bird1	bird2	bird3	bird4	bird1	bird2	bird3	bird4	bird1	bird2	bird3	bird4	bird1	bird2	bird3	bird4	bird1	bird2	bird3	bird4
<i>N</i> -EtFOSE	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
PFBS	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
PFHxS	1.20	2.02	1.55	4.12	2.42	2.12	3.67	2.67	9.74	5.37	2.53	2.27	0.82	0.67	1.07	1.05	0.84	1.41	1.53	1.38
PFHpS	<MQL	<MQL	4.77	1.71	<MQL	<MQL	1.71	<MQL	2.56	1.45	1.42	0.98	0.42	0.26	0.73	0.49	0.39	1.30	0.98	0.81
PFOS	19.08	98.62	53.94	177.69	212.83	156.29	251.45	110.23	63.74	90.36	61.65	58.59	24.27	17.85	35.34	35.78	37.08	71.04	102.17	77.03
PFDS	<MQL	0.37	0.44	0.40	<MQL	<MQL	0.40	<MQL	0.49	0.37	0.45	0.28	0.12	<MQL	0.16	0.10	<MQL	<MQL	0.35	<MQL
PFHpA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.12	n.d.	<MQL	<MQL	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
PFOA	<MQL	0.60	n.a.	1.80	0.98	0.59	1.30	1.02	3.24	5.42	6.67	3.06	0.46	0.25	0.41	0.40	0.55	0.64	0.56	0.62
PFNA	2.17	3.91	3.87	2.36	5.11	2.93	3.89	1.97	5.35	3.45	1.65	1.18	0.76	0.74	0.94	0.70	1.25	1.74	1.61	0.92
PFDA	0.42	1.24	0.70	0.66	1.14	0.86	1.54	0.41	1.06	0.72	0.55	0.33	0.24	0.19	0.25	0.19	<MQL	0.46	0.61	0.40
PFUnDA	3.39	9.75	6.87	4.49	5.07	4.21	10.00	2.57	10.21	4.95	7.88	2.79	1.01	0.94	2.17	1.59	2.10	3.58	5.53	2.05
PFDoDA	1.36	2.45	1.97	1.51	1.64	1.61	2.57	0.85	2.57	1.47	2.55	1.21	0.49	<MQL	0.91	0.55	1.18	1.58	2.50	1.06
PFTriDA	3.11	3.03	3.48	3.04	2.92	3.12	4.34	1.86	7.34	2.62	5.05	2.13	1.04	0.67	0.93	0.70	1.66	3.67	5.15	2.69
PFTeDA	0.60	0.74	0.80	1.20	0.78	0.70	0.90	n.a.	1.37	0.79	0.86	0.73	n.d.	n.d.	n.d.	n.d.	0.62	0.69	1.14	0.80
PFHxDA	n.d.	n.d.	n.d.	<MQL	0.11	n.d.	<MQL	n.d.	<MQL	<MQL	<MQL	<MQL	n.d.	n.d.	n.d.	n.d.	<MQL	<MQL	<MQL	<MQL
PFOcDA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
PFOSA	10.78	29.78	17.75	42.67	23.31	14.47	18.19	16.60	39.45	18.34	12.17	17.04	8.32	4.76	6.64	12.66	6.67	8.63	11.66	16.15
<i>N</i> -MeFOSA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
<i>N</i> -EtFOSA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
<i>N</i> -MeFOSE	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
<i>N</i> -EtFOSE	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

Table A9. Mean PFC concentrations (ng g⁻¹ wet weight) of red-throated divers (n = 4) and absolute standard deviation (ng g⁻¹ wet weight) for blood, brain, fatty tissue, gall bladder, heart, kidney, liver, lung, muscle and spleen

Compound	Blood		Brain		Fatty tissue		Gall bladder		Heart		Kidney		Liver		Lung		Muscle		Spleen	
	Mean	s.d.	Mean	s.d.	Mean	s.d.	Mean	s.d.	Mean	s.d.	Mean	s.d.	Mean	s.d.	Mean	s.d.	Mean	s.d.	Mean	s.d.
PFBS	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
PFHxS	4.38	2.53	0.97	0.40	1.23	0.99	3.00	0.69	2.09	0.42	2.22	1.31	2.72	0.67	4.98	3.47	0.90	0.19	1.29	0.31
PFHpS	0.79	0.07	0.39	0.19	n.d.	n.d.	1.55	0.00	0.75	0.27	3.24	2.17	1.71	0.00	1.60	0.67	0.47	0.19	0.87	0.38
PFOS	73.14	26.01	40.36	11.69	54.38	42.09	84.50	46.75	72.21	18.83	87.33	68.47	182.70	62.14	68.58	14.67	28.31	8.77	71.83	26.81
PFDS	0.23	0.00	0.53	0.12	n.d.	n.d.	0.29	0.00	<MQL	<MQL	0.41	0.03	0.40	0.00	0.40	0.09	0.13	0.03	0.35	0.00
PFHpA	0.08	0.00	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.12	0.00	n.d.	n.d.		
PFOA	0.98	0.48	0.38	0.18	0.26	0.13	0.68	0.45	0.73	0.08	1.20	0.85	0.97	0.29	4.60	1.75	0.38	0.09	0.59	0.05
PFNA	2.03	0.67	0.80	0.34	1.35	0.00	2.60	1.38	1.97	0.80	3.08	0.94	3.48	1.34	2.91	1.90	0.79	0.11	1.38	0.37
PFDA	0.43	0.08	0.43	0.16	0.26	0.03	0.68	0.31	0.48	0.14	0.76	0.35	0.99	0.47	0.67	0.31	0.22	0.03	0.49	0.11
PFUnDA	3.80	1.13	5.62	2.54	1.08	0.68	4.50	3.39	2.72	0.64	6.12	2.82	5.46	3.20	6.46	3.26	1.43	0.58	3.31	1.64
PFDoDA	1.12	0.35	3.17	1.39	0.54	0.00	2.62	0.00	1.03	0.27	1.82	0.49	1.67	0.70	1.95	0.71	0.65	0.23	1.58	0.65
PFTriDA	1.80	0.42	8.62	3.42	0.77	0.07	2.11	1.03	1.95	0.43	3.16	0.21	3.06	1.01	4.28	2.40	0.84	0.18	3.29	1.49
PFTeDA	0.35	0.12	2.32	1.08	n.d.	n.d.	0.51	0.11	n.d.	n.d.	0.84	0.25	0.79	0.11	0.94	0.29	n.d.	n.d.	0.81	0.23
PFHxDA	n.d.	n.d.	<MQL	<MQL	n.d.	n.d.	n.d.	n.d.	<MQL	<MQL	n.d.	n.d.	0.11	0.00	<MQL	<MQL	n.d.	n.d.	<MQL	<MQL
PFOcDA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
PFOSA	21.53	16.75	12.41	7.40	13.54	3.49	16.80	6.54	13.71	5.54	25.25	14.02	18.14	3.76	21.75	12.10	8.10	3.38	10.78	4.13
N-MeFOSA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
N-EtFOSA	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
N-MeFOSE	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
N-EtFOSE	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

Recovery rates of the complete method**Table A10. Target analytes, their average absolute recovery rates ($n = 3$) for the complete method including sample processing and standard addition method as well as the relative standard deviations**

Recovery rates were calculated on the basis of a matrix assisted calibration. The sample processing as well as the matrix assisted calibration were performed in extracts of uncontaminated turkey liver used as a ‘comparable’ matrix. n.a., not analysed

Compound	Recovery rate (%)	Relative standard deviation (%)
PFBS	97.1	38.6
PFHxS	114.3	47.5
PFHpS	108.4	31.6
PFOS	98.3	48.1
PFDS	113.4	57.6
PFHpA	109.1	49.0
PFOA	109.4	29.3
PFNA	110.7	37.1
PFDA	88.8	42.7
PUnDA	93.3	37.9
PDoDA	105.1	31.3
PTriDA	109.9	44.3
PTeDA	98.0	17.9
PFHxDA	n.a.	n.a.
PFocDA	84.7	12.0
PFOSA	94.8	56.1
<i>N</i> -MeFOSA	99.4	24.6
<i>N</i> -EtFOSA	157.8	93.9
<i>N</i> -MeFOSE	106.4	24.9
<i>N</i> -EtFOSE	127.4	35.7

Details of factor analysis

Table A11. Variables, factor loadings and communalities of the factor analysis as well as eigenvalues and explained variance (%) of the three factors

Variable	Loading Factor 1	Loading Factor 2	Loading Factor 3	Communality
PFHxS			0.829	0.786
PFHpS		0.416	0.524	0.493
PFOS ^A		0.897		0.807
PFDS	0.919			0.928
PFOA			0.920	0.873
PFNA		0.793	0.495	0.878
PFDA		0.884		0.928
PFUnDA	0.650	0.589		0.966
PFDoDA	0.933			0.948
PFTriDA	0.970			0.956
PFTeDA	0.937			0.879
eigenvalue	5.73	2.51	1.31	
Explained variance (%)	52.1	22.8	10.3	

^ACombined variable from PFOS and PFOSA.

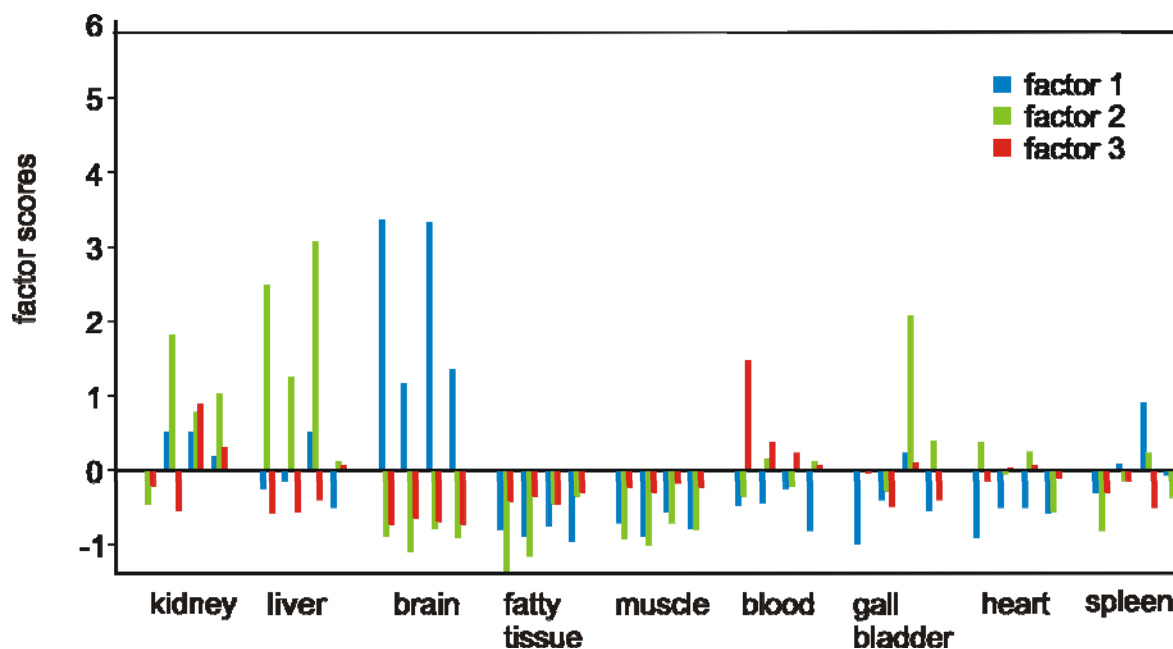


Fig. A2. Factor scores of nine different tissue samples of red-throated divers ($n = 4$). For the factor analysis the Kaiser criterion was used so that only eigenvalues greater than 1 were applied. Varimax rotation was performed.

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