

Supplementary Materials: Rapid Determination of Per- and Polyfluoroalkyl Substances (PFAS) in Harbour Porpoise Liver Tissue by HybridSPE®-UPLC®-MS/MS

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Table S1. SRM (Selected Reaction Monitoring) transitions, collision energies, and cone voltage values for the UPLC®-MS/MS analysis of PFAS.

Target Analytes	Transition 1*	Transition 2	Collision energy (V)	Cone voltage values (V)	Ion ratio % [#]
PFBS	299>80	299>299	26; 24	22; 8	172
PFHxS	399>80	399>399	34; 34	50; 8	69.8
PFOS	499>99	499>80	44; 44	56; 36	89.8
PFPeA	263>219	-	8	20	-
PFHxA	313>269	313>119	8;18	10;10	4.20
PFHpA	363>169	363>319	16;10	16;16	35.0
PFOA	413>369	413>169	8;18	20;20	27.1
PFNA	463>419	463>219	10;16	20;20	19.1
PFDA	513>469	513>269	10;18	16;16	11.1
PFUnA	563>519	563>269	10;18	12;12	12.7
PFDoA	613>569	613>169	12;26	26;26	12.1
PFTTrA	663>619	663>169	12;24	28;28	12.9
PFTeA	713>669	713>169	14;30	20;20	13.9
PFOSA	498>78	498>478	28;28	12;12	6.3
EtFOSA	526>169	526>219	44;44	26;26	69.6
PFOA-C ¹³	421>172	421>223	16;16	16;16	-
PFOS-C ¹³	507>80	507>172	56;56	46;32	-

* Ion transition with higher signal intensity (used as the quantification ion).

[#] Calculated from the replicates ($N = 5$) performed in a standard solvent solution (10 ng/mL).

Table S2. Retention (RT) and relative retention (RRT) times of the UPLC®-MS/MS method, and presenting the internal standard (IS) used for the quantification of every target analyte.

Target Analytes	RT (min)	RRT	IS
PFBS	1.69	0.80	PFOA- ¹³ C
PFHxS	1.97	0.95	PFOA- ¹³ C
PFOS	2.20	1.00	PFOS- ¹³ C
PFPeA	1.63	0.78	PFOA- ¹³ C
PFHxA	1.83	0.88	PFOA- ¹³ C
PFHpA	1.98	0.95	PFOA- ¹³ C
PFOA	2.09	1.00	PFOA- ¹³ C
PFNA	2.19	1.00	PFOS- ¹³ C
PFDA	2.28	1.04	PFOS- ¹³ C
PFUnA	2.38	1.08	PFOS- ¹³ C
PFDoA	2.46	1.12	PFOS- ¹³ C
PFTTrA	2.54	1.16	PFOS- ¹³ C
PFTeA	2.61	1.19	PFOS- ¹³ C
PFOSA	2.48	1.11	PFOS- ¹³ C
EtFOSA	2.71	1.24	PFOS- ¹³ C
PFOA- ¹³ C	2.09	-	-
PFOS- ¹³ C	2.19	-	-

Table S3. Mean absolute and relative recoveries (%; $N=4$) of the target analytes at a fortified amount of 10 ng with 0.001 % (w/v) ammonium formate in methanol as the precipitation agent.

Target analyte [IS used for the calculation of the relative recovery (%)]	Absolute recovery (%)	Relative recovery (%)
PFPA (PFOA- ^{13}C)	76.2	98.7
PFHxA (PFOA- ^{13}C)	44.4	148.1
PFHpA (PFOA- ^{13}C)	87.3	113.1
PFOA (PFOA- ^{13}C)	84.8	109.9
PFNA (PFOS- ^{13}C)	84.7	121.1
PFDA (PFOS- ^{13}C)	79.3	115.9
PFUnA (PFOS- ^{13}C)	81.0	122.0
PFDoA (PFOS- ^{13}C)	85.0	113.2
PFTTrA (PFOS- ^{13}C)	82.8	112.0
PFTeA (PFOS- ^{13}C)	89.4	117.5
PFBS (PFOA- ^{13}C)	83.6	108.2
PFHxS (PFOA- ^{13}C)	80.9	104.6
PFOS (PFOS- ^{13}C)	54.0	131.2
PFOSA (PFOS- ^{13}C)	81.1	115.8
EtFOSA (PFOS- ^{13}C)	83.0	116.8