

## Accessory publication

**Environmental levels and distribution of structural isomers of perfluoroalkyl acids after aqueous fire-fighting foam (AFFF) contamination**A. Kärrman,<sup>A,C</sup> K. Elgh-Dalgren,<sup>A</sup> C. Lafossas<sup>A</sup> and T. Møskeland<sup>B</sup><sup>A</sup>Man-Technology-Environment Research Centre, School of Science and Technology, Örebro University, SE-701 82 Örebro, Sweden.<sup>B</sup>Det Norske Veritas (DNV), Veritasveien 1, 1322 Høvik, Norway.<sup>C</sup>Corresponding author. Email: anna.karrman@oru.se**Table A1. Abbreviation, chemical formula and structure of PFOS and PFOA isomers**

Abbreviation	Formula	Name
L-PFOS	$\text{CF}_3\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{SO}_3^-$	<i>n</i> -perfluoro-octanesulfonate
1-PFOS	$\text{CF}_3\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}(\text{CF}_3)\text{SO}_3^-$	perfluoro-1-methyl-heptanesulfonate
2-PFOS	$\text{CF}_3\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}(\text{CF}_3)\text{CF}_2\text{SO}_3^-$	perfluoro-2-methyl-heptanesulfonate
3-PFOS	$\text{CF}_3\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{SO}_3^-$	perfluoro-3-methyl-heptanesulfonate
4-PFOS	$\text{CF}_3\text{CF}_2\text{CF}_2\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{CF}_2\text{SO}_3^-$	perfluoro-4-methyl-heptanesulfonate
5-PFOS	$\text{CF}_3\text{CF}_2\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{SO}_3^-$	perfluoro-5-methyl-heptanesulfonate
6-PFOS	$\text{CF}_3\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{SO}_3^-$	perfluoro-6-methyl-heptanesulfonate
4,4-PFOS	$\text{CF}_3\text{CF}(\text{CF}_3)_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{SO}_3^-$	perfluoro-4,4-dimethyl-hexanesulfonate
3,5-PFOS	$\text{CF}_3\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{SO}_3^-$	perfluoro-3,5-dimethyl-hexanesulfonate
4,5-PFOS	$\text{CF}_3\text{CF}(\text{CF}_3)\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{CF}_2\text{SO}_3^-$	perfluoro-4,5-dimethyl-hexanesulfonate
5,5-PFOS	$\text{CF}_3\text{C}(\text{CF}_3)_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{SO}_3^-$	perfluoro-5,5-dimethyl-hexanesulfonate
L-PFOA	$\text{CF}_3\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{COOH}$	<i>n</i> -perfluoro-octanoic acid
2-PFOA	$\text{CF}_3\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}(\text{CF}_3)\text{COOH}$	perfluoro-2-methyl-heptanoic acid
3-PFOA	$\text{CF}_3\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}(\text{CF}_3)\text{CF}_2\text{COOH}$	perfluoro-3-methyl-heptanoic acid
4-PFOA	$\text{CF}_3\text{CF}_2\text{CF}_2\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{COOH}$	perfluoro-4-methyl-heptanoic acid
5-PFOA	$\text{CF}_3\text{CF}_2\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{CF}_2\text{COOH}$	perfluoro-5-methyl-heptanoic acid
6-PFOA	$\text{CF}_3\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{COOH}$	perfluoro-6-methyl-heptanoic acid
4,4-PFOA	$\text{CF}_3\text{CF}_2\text{CF}(\text{CF}_3)_2\text{CF}_2\text{CF}_2\text{COOH}$	perfluoro-4,4-dimethyl-hexanoic acid
3,5-PFOA	$\text{CF}_3\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}(\text{CF}_3)\text{CF}_2\text{COOH}$	perfluoro-3,5-dimethyl-hexanoic acid
4,5-PFOA	$\text{CF}_3\text{CF}(\text{CF}_3)\text{CF}(\text{CF}_3)\text{CF}_2\text{CF}_2\text{COOH}$	perfluoro-4,5-dimethyl-hexanoic acid
5,5-PFOA	$\text{CF}_3\text{C}(\text{CF}_3)_2\text{CF}_2\text{CF}_2\text{CF}_2\text{COOH}$	perfluoro-5,5-dimethyl-hexanoic acid

**Table A2. Recoveries (%) and standard deviations of spiked native compounds to different matrices ( $n = 3$ )**

Numbers marked in italics are compounds that were not quantified in respective matrix because of ionisation effects or low recoveries

	Sediment		Water		Mussel		Fish liver	
	Average	s.d.	Average	s.d.	Average	s.d.	Average	s.d.
6:2 FTS	120	15.9	114	0.25	<i>541</i>	<i>4.20</i>	<i>436</i>	<i>24.4</i>
PFBS	86	11.5	122	33.9	102	21.3	78	27.2
PFHxS	77	3.46	93	2.25	110	6.49	99	3.97
PFOS	89	4.06	103	3.02	102	2.82	98	4.88
PFDS	84	7.00	74	16.2	64	8.22	44	2.43
PFPeA	40	0.90	93	0.34	110	0.55	116	8.28
PFHxA	47	1.84	97	1.20	102	2.73	96	1.52
PFHpA	38	3.03	69	38.6	35	5.38	66	29.7
PFOA	47	1.54	99	0.69	103	7.72	96	1.16
PFNA	68	8.80	103	0.01	117	0.80	105	23.9
PFDA	<i>15</i>	<i>12.8</i>	97	1.78	100	0.41	98	3.77
PFUnDA	70	9.3	96	0.12	113	4.63	100	8.17
PFDoDA	62	9.7	80	14.1	64	6.88	53	3.96
PFTTrDA	70	14.4	57	13.2	24	5.58	24	1.18
PFTeDA	67	11.2	54	13.8	9	2.45	9	<i>1.07</i>

**Table A3. Recoveries (%) and standard deviations of labelled compounds added as internal standards to the studied samples**

NQ, not quantified because of ionisation effects

	Soil ( <i>n</i> = 10)		Sediment ( <i>n</i> = 9)		Water ( <i>n</i> = 3)		Mussel ( <i>n</i> = 3)		Crab ( <i>n</i> = 4)		Fish liver ( <i>n</i> = 4)	
	Average	s.d.	Average	s.d.	Average	s.d.	Average	s.d.	Average	s.d.	Average	s.d.
PFHxS	60	10.8	70	6.89	62	21.0	80	4.26	51	4.27	57	8.41
PFOS	31	17.0	58	5.32	52	7.53	77	34.0	107	44.8	21	15.8
PFHxA	39	11.1	54	7.63	85	8.53	96	12.6	99	37.5	93	20.4
PFOA	52	18.2	57	6.07	86	14.6	87	5.23	77	14.8	87	18.8
PFNA	30	13.2	54	13.5	62	3.76	152	68.6	163	57.9	38	25.7
PFDA	NQ	NQ	38	11.9	132	28.7	84	37.2	146	80.0	94	73.9
PFUnDA	25	10.7	36	13.4	117	26.1	98	38.1	121	63.5	61	46.7
PFDoDA	26	10.8	28	11.9	62	21.0	80	4.26	51	4.27	57	8.41

**Table A4. Recoveries (%) and standard deviations of PFOS isomers in a Fluka standard spiked to sediment (*n* = 3) and water (*n* = 3)**

Chromatographic separation was performed for 1/2/6-PFOS and 3,5/4,5/5,5-PFOS using the quantification method thus not separating all isomers

	L-PFOS		1/2/6-PFOS		3/4/5-PFOS		3,5/4,5/5,5-PFOS		4,4-PFOS	
	Average	s.d.	Average	s.d.	Average	s.d.	Average	s.d.	Average	s.d.
Sediment	64.1	3.13	54.9	4.10	56.6	5.30	50.6	7.63	59.7	16.0
Water	87.2	3.63	82.4	2.34	84.1	4.39	85.3	6.95	86.4	8.99

**Table A5. Concentration (ng g<sup>-1</sup> DW) of PFAAs and 6:2 FTS in soil with increasing distance from a fire-fighting training platform at Flesland**

NQ, not quantified because of ionisation effects. Data marked with an asterisk (\*) were quantified with a higher uncertainty because of ionisation effects (recovery between 10 and 20%)

	0 m	10 m	20 m	30 m	40 m	50 m	75 m	100 m	150 m	200 m
Dry weight (%)	92%	73%	67%	78%	64%	67%	71%	80%	57%	58%
6:2 FTS	612*	2101*	751*	329*	38	5.2	7.7	9.2	2.5	0.84
PFBS	0.29	1.4	1.8	1	0.67	0.28	<0.11	<0.11	<0.11	<0.11
PFHxS	6.2	17	21	15	5.2	5.3	1.1	0.54	0.64	0.12
PFOS	273*	1905*	705*	331*	129	96	24	6.1	7.6	1.6
PFDS	3.2*	54*	8.5*	4*	2.8	1.1	0.36	0.19	0.13	<0.10
PFPeA	0.68	7	17	28	17	11	8.8	3.7	0.88	0.52
PFHxA	2.5	8.1	10.2	18.5	11.5	6.8	3.6	1.5	0.32	0.18
PFHpA	0.8	4.5	2.8	4.6	6.7	2.3	1.8	0.77	0.27	0.19
PFOA	1.4	7.7	4.4	4.4	12.2	2.7	1.2	0.54	0.36	0.23
PFNA	<1.0	NQ	NQ	1.7*	6.4	<1.0	<1.0	<1.0	<0.60	<0.70
PFDA	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ
PFUnDA	0.94	5.8*	1.6*	<1.5	3.7	0.48	<0.1	<0.5	<0.5	<0.5
PFDoDA	0.58	3.77*	NQ	NQ	4.1	0.6	<0.1	0.13	0.17	<0.1
PFTTrDA	<0.1	0.25*	<0.1	0.14*	0.32	0.32	<0.1	<0.1	<0.1	<0.1
PFTeDA	<0.1	<0.1	<0.1	<0.1	<0.3	<0.1	<0.11	<0.1	<0.1	<0.1

**Table A6. Concentration (ng g<sup>-1</sup> DW) of PFAAs and 6:2 FTS in sediment samples from Lake Langavatn near the fire-fighting training platform at Flesland**

NQ, not quantified because of ionisation effects or low recoveries

	1:1	1:2	1:3	2:1	2:2	2:3	3:1	3:2	3:3
Dry weight (%)	8.2%	8.5%	9.2%	7.0%	8.1%	12%	12%	12%	13%
6:2 FTS	9.1	8.4	9.8	12	7.8	1.5	4.1	7.3	8.7
PFBS	<0.11	0.17	<0.11	<0.14	<0.14	<0.10	<0.10	<0.10	<0.10
PFHxS	2.2	2.4	2.6	1.4	1.3	0.8	0.65	NQ	0.7
PFOS	70	49	70	88	85	35	49	57	53
PFDS	0.89	0.22	0.42	<0.21	0.38	<0.13	1.7	1.3	0.4
PFPeA	0.91	0.52	0.69	0.69	<0.57	0.42	0.78	0.57	0.37
PFHxA	1.3	0.7	0.9	0.76	<0.6	0.58	1.6	0.7	0.45
PFHpA	0.32	0.2	0.28	<0.1	<0.5	<0.5	0.15	0.17	0.17
PFOA	<0.5	<0.5	<0.5	<0.75	<0.75	<0.75	<0.5	<0.5	<0.5
PFNA	<2.5	<2.5	<2.5	<3.2	<2.8	<1.9	<1.8	<1.9	<1.8
PFDA	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ
PFUnDA	11	9.8	4.9	NQ	23	0.56	21	26	25
PFDoDA	0.5	<0.5	<0.5	NQ	0.3	<0.11	0.76	0.96	0.18
PFTTrDA	3.2	0.81	0.77	<0.1	2.5	<0.1	7.9	11	0.9
PFTeDA	<0.28	<0.28	<0.28	<0.36	<0.31	<0.21	<0.20	<0.21	<0.20

**Table A7. Concentration (ng L<sup>-1</sup>) of PFAAs and 6:2 FTS in seepage water samples taken from the fire-fighting training platform at Flesland**

Analysed with two different mass spectrometers, diluted 5 times on QPXE, and 100 times on Xevo TQS.

IDL Instrument detection limit, was not established on the Xevo instrument

	QPXE			Xevo		
	1	2	3	1 (100×)	2 (100×)	3 (100×)
6:2 FTS	6693	5254	5110	4983	3878	4334
PFBS	74	68	148	74	52	53
PFHxS	471	413	319	540	400	392
PFOS	2078	1581	1427	1890	1491	1371
PFDS	<0.41	<0.39	<0.38	0.13	<IDL	<IDL
PFPeA	631	552	498	775	661	586
PFHxA	554	439	385	561	455	424
PFHpA	205	177	172	215	180	176
PFOA	191	143	130	189	145	140
PFNA	33	22	30	36	27	26
PFDA	4.2	3.4	3.7	5.3	4.4	4.2
PFUnDA	17	9.1	6.8	18	8.7	8.6
PFDoDA	<0.62	<0.58	<0.57	1.1	1.7	0.67
PFTTrDA	<0.60	<0.27	<0.27	<IDL	<IDL	0.54
PFTeDA	<0.29	<0.27	<0.27	3.5	<IDL	<IDL

**Table A8. Concentration (ng g<sup>-1</sup> FW) of PFAAs and 6:2 FTS in biota samples from Lake Langavatn (trout liver) and receiving sea (crab and mussel) near a fire-fighting training platform at Flesland**

NQ, not quantified because of ionisation effects; Det, detected but not quantified because of ionisation effects. Data marked with an asterisk (\*) were quantified with a higher uncertainty because of ion suppression (recovery between 10 and 20%)

	Mussel	Mussel	Mussel	Crab	Crab	Crab	Crab	Trout liver	Trout liver	Trout liver	Trout liver
	1	2	3	1	2	3	4	1	2	3	4
6:2 FTS	NQ	NQ	NQ	NQ	NQ	NQ	NQ	Det	Det	Det	Det
PFBS	<0.10	<0.10	<0.10	<0.20	<0.10	<1.3	<0.10	<0.05	<0.05	<0.30	<0.30
PFHxS	<0.05	<0.05	<0.05	0.46	0.28	0.12	<0.10	268	132	118	123
PFOS	<0.15	<0.15	<0.15	1	4.9*	2.3	0.8	2103	2407	2082	2532
PFDS	<0.05	<0.05	<0.05	<0.05	0.56	0.17	0.13	65	37	57	49
PFPeA	<0.20	<0.50	<0.50	<0.30	<0.20	<0.97	<0.20	<0.96	<0.20	<0.51	<0.50
PFHxA	<0.30	<1.0	<1.0	<0.10	<0.29	<0.16	<0.30	<0.15	0.24	<0.2	<0.15
PFHpA	<0.05	<0.05	<0.05	<0.05	<0.05	<0.10	<0.05	<0.10	<0.05	<0.07	<0.05
PFOA	<0.07	<0.08	<0.08	0.82	<0.70	<0.10	0.16	0.49	<0.40	<0.60	<0.20
PFNA	<0.10	<0.10	<0.10	0.12	<0.30	<0.23	<0.20	NQ	4	NQ	NQ
PFDA	<0.10	<0.10	<0.10	<0.20	<0.20	<0.20	<0.20	14	10*	11	11
PFUnDA	<0.10	<0.10	<0.10	0.51	<1.0	1.2	0.72	140	81	95	89
PFDoDA	<0.10	<0.10	<0.10	0.42	<0.5	<0.5	0.24	14	5.6	5.6	4.7
PFTTrDA	0.47	0.38	0.38	1.1	1.2*	2.0	0.95	83	39	28	24
PFTeDA	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ

**Table A9. Percentage of the total concentration (ng g<sup>-1</sup> DW) of PFOS isomers in soil taken with increasing distance to a fire-fighting training area in Flesland**

Missing values are non-detections, generally below 0.1%

	L-PFOS	1-PFOS	2-PFOS	6-PFOS	3/4/5-PFOS	3,5-PFOS	4,5/5,5-PFOS	4,4-PFOS
0 m	63	5.1	0.98	13	17	0.46	0.07	0.49
10 m	71	3.7	0.72	12	13	0.27	0.23	
40 m	80	2.4	0.45	8.0	8.6	0.14	0.18	
75 m	79	2.9	0.34	8.2	8.7	0.13	0.19	
100 m	85	1.2	0.55	5.8	6.7		0.16	
150 m	71	3.3	0.82	11	13	0.37	0.54	
200 m	84	1.9		4.6	9.1	0.21		

**Table A10. Percentage of the total concentration (ng g<sup>-1</sup> DW) of PFOS isomers in seepage water from the fire-fighting training area in Flesland and sediment in the receiving Lake Langavatnet**

Missing values are non-detections, generally below 0.1%

	L-PFOS	1-PFOS	2-PFOS	6-PFOS	3/4/5-PFOS	3,5-PFOS	4,5/5,5-PFOS	4,4-PFOS
Water	61	4.6	1.0	14	18	0.49	0.61	0.10
Water	60	4.7	1.1	15	18	0.47	0.57	0.07
Water	58	5.4	1.3	15	19	0.52	0.65	0.09
Sediment 1:1	77	2.4	0.67	9.2	10	0.19	0.21	
Sediment 2:1	77	3.4	0.57	9.4	9.5	0.17	0.19	
Sediment 3:1	85	1.3	0.52	7.2	5.8	0.10	0.13	



**Table A11. Percentage of the total concentration (ng g<sup>-1</sup> DW) of PFOA isomers in soil taken with increasing distance to a fire-fighting training area in Flesland**

Missing values are non-detections, generally below 0.1%

	L-PFOA	2-PFOA	3/4/6-PFOA	5-PFOA	3,5-PFOA	4,5-PFOA	4,4-PFOA	5,5-PFOA
0 m	80.5		12.7	6.7				
10 m	85.2		8.9	4.4			1.6	
40 m	94.1		1.9	0.86	0.20		3.0	
75 m	100							
100 m	100							
150 m	100							
200 m	100							

**Table A12. Percentage of the total concentration (ng g<sup>-1</sup> DW) of PFOA isomers in seepage water from the fire-fighting training area in Flesland**

Missing values are non-detections, generally below 0.1%

	L-PFOA	2-PFOA	3/4/6-PFOA	5-PFOA	3,5-PFOA	4,5-PFOA	4,4-PFOA	5,5-PFOA
Water	72		14	13	0.36			0.14
Water	76		15	8.1	0.42	0.28		0.12
Water	75		14	10				0.29

**Table A13. Percentage of the total concentration (ng g<sup>-1</sup> DW) of PFOS isomers in Trout liver from Lake Langavatnet**

Missing values are non-detections, generally below 0.1%

	L-PFOS	1-PFOS	2-PFOS	6-PFOS	3/4/5-PFOS	3,5-PFOS	4,5/5,5-PFOS	4,4-PFOS
Fish	87	2.2	0.32	5.7	5.0			
Fish	90	1.6	0.19	4.8	3.7			
Fish	89	2.0	0.23	4.3	4.1			
Fish	88	2.3	0.28	5.1	4.2			