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SUPPLEMENTARY MATERIAL

Distribution of poly- and perfluoroalkyl substances in pig liver and muscle: implications for food safety

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Supplementary Table 1. Tandem mass spectrometry instrumental conditions.

Parameter	Mode/Value
Ionisation	ESI-
Analysis mode	MRM
Cone voltage	31 V
Capillary	0.50 KV
Source temperature	150°C
Desolvation temperature	500°C
Desolvation flow	900 L/h
Cone gas	50 L/h
Collision energy	15 eV
Extractor	1 V
RF Lens	0.2 V

MRM, multiple reaction monitoring; ESI, negative electrospray ionisation.

Supplementary Table 2. Analyte identification and tandem mass spectrometry transition parameters for target per- and polyfluoroalkyl substances.

Analyte	Acronym	MRM-transition	Cone voltage (V)	Collision energy (eV)
Perfluoro-n-[1.2-$^{13}C_2$]octanoic acid	M2PFOA	**415.00>370.00**	20	9
Sodium perfluoro-1-[1.2.3.4-$^{13}C_4$]octanesulfonate	MPFOS	**503.00>80.00**	30	45
N-methyl-d_3-perfluoro-1-octanesulfonamidoacetic acid	d3-N-MeFOSAA	**573.00>419.00**	25	20
Perfluorohexanoic acid	PFHxA	**313.00>269.00** 313.00>118.94	20	7 20
Ammonium perfluoro(2-methyl-3-oxa)hexanoate	HFPO-DA	**285.00>169.00** 285.00>119.00	12	8 28
Perfluoroheptanoic acid	PFHpA	**363.00>319.00** 363.00>169.00	15	8 16
Sodium dodecafluoro-3H-4.8-dioxanonanoate	NaDONA	**377.00>250.96** 377.00>84.93	22	10 28
Potassium perfluorobutanesulfonate	PFBS	**299.00>79.85** 299.00>98.85	28	30 25
Sodium perfluorohexanesulfonate	PFHxS	**399.00>79.91** 399.00>98.91	16	36 32
Perfluorooctanoic acid	PFOA	**413.00>369.00** 413.00>169.00	20	9 18
Perfluorononanoic acid	PFNA	**463.00>419.00** 463.00>219.00	20	9 15
Perfluorooctanesulfonic acid	PFOS	**499.00>80.00** 499.00>98.91	30	45 35
Perfluorodecanoic acid	PFDA	**513.00>469.00** 513.00>219.00	20	10 18
N-Methyl perfluorooctanesulfonamidoacetic acid	N-MeFOSAA	**570.00>419.00** 570.00>219.00	30	18 25
Perfluoroundecanoic acid	PFUdA	**563.00>519.00** 563.00>269.00	20	10 18
Perfluorododecanoic acid	PFDoA	**613.15>569.00** 613.15>169.00	28	10 26

The transitions in bold are those used for quantification. MRM, multiple reaction monitoring.

Supplementary Table 3. Method performance assessment (BCC-back-calculated concentration, trueness, intermediate precision).

Analyte	Range BCC (±%)		
	Liver	*Semimembranosus*	*Longissimus dorsi*
PFHxA	-2/+2	-3/+2	-6/+4
HFPO-DA	-1/+1	-4/+5	-4/+3
PFHpA	-3/+3	-13/+14	-5/+4
NaDONA	-13/+2	-4/+2	-5/+7
PFBS	-3/+3	-11/+5	-9/+7
PFHxS	-5/+9	-6/+7	-6/+10
PFOA	-3/+2	-10/+5	-7/+3
PFNA	-8/+4	-3/+4	-2/+3
PFOS	-2/+4	-5/+5	-6/+10
PFDA	-4/+3	-4/+3	-5/+4
N-MeFOSAA	-9/+6	-8/+6	-5/+7
PFUdA	-6/+5	-7/+7	-6/+12
PFDoA	-5/+4	-9/+8	-4/+2

Analyte	Trueness (% bias)											
	Intra-day range						Inter-day					
	Liver		*Semimembranosus*		*Longissimus dorsi*		Liver		*Semimembranosus*		*Longissimus dorsi*	
	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)
PFHxA	+7/+10	+2	+8/+12	-2/0	+8/+13	+2	+8	+2	+10	-1	+10	+2
HFPO-DA	+4/+5	-1	+6/+8	0/+4	+3/+4	0	+4	-1	+7	+2	+4	0
PFHpA	+2/+4	0/+2	+15/+19	-1	+1/+4	+1/+2	+3	+1	+17	-1	+3	+1
NaDONA	-8/-6	-7/-3	+7/+10	-6/-5	0/+2	-1/0	-7	-5	+9	-5	+1	-1
PFBS	+2/+4	-2/+5	+1/+7	-5/-3	+5/+7	-1/0	+3	+2	+4	-4	+6	0
PFHxS	+4/+6	-1/+1	+4/+6	-7	+8/+9	-1/0	+5	0	+5	-7	+9	-1
PFOA	+8/+9	-1/+1	+9	-3/-1	+5/+6	+1/+2	+8	0	+9	-2	+5	+2
PFNA	+6/+9	+1/+2	+10	-1/0	+7/+9	-1/+1	+7	+1	+10	0	+8	0
PFOS	+10/+14	-1/+3	+5/+7	-4/-2	+8	+2	+12	+1	+6	-3	+8	+2
PFDA	+5/+17	-1	+8/+12	-2/0	+4	0/+3	+11	-1	+10	-1	+4	+1
N-MeFOSAA	-14/-10	-20/-11	+9/+15	-7/-6	+4/+12	-18/-12	-12	-15	+12	-7	+8	-15
PFUdA	+8/+14	+1/+3	+10/+12	-17/-15	+6/+9	+2/+4	+11	+2	+11	-16	+8	+3
PFDoA	+3/+10	-1/+2	+2/+6	-8/-5	+2	-3/-1	+7	0	+4	-7	+2	-2

Analyte	Intermediate precision (%)											
	Intra-day range						Inter-day					
	Liver		*Semimembranosus*		*Longissimus dorsi*		Liver		*Semimembranosus*		*Longissimus dorsi*	
	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)	QC 0.040 (µg/kg)	QC 0.200 (µg/kg)
PFHxA	8-9	4-5	2-4	2-3	3-7	2-3	8	4	3	2	5	2
HFPO-DA	6-13	4-6	3-6	1-4	6-7	2-4	9	4	4	4	6	3
PFHpA	6-7	2-3	2-4	4	2-5	2	6	2	3	3	4	2
NaDONA	3-5	4-10	5	4-5	8-9	3-5	4	7	5	4	8	3
PFBS	4-5	3-8	4-5	3-8	4-5	2-3	4	6	5	6	4	2
PFHxS	7-9	4-5	4-10	2	3-4	2-4	7	4	7	2	3	3
PFOA	6-7	2-4	2-3	3-4	3-6	3	6	3	3	3	4	3
PFNA	4-8	1-2	4-5	1-4	3-4	1-2	6	1	4	2	3	2
PFOS	4-5	3	3-5	3	4-6	1-2	4	3	4	3	4	2
PFDA	5-8	2	3	3	5	1	8	3	3	3	5	2
N-MeFOSAA	2-18	2-8	4	3-10	2-3	6-8	12	8	4	7	4	7
PFUdA	2-9	3-4	3-6	4-5	1-6	2	6	3	4	4	4	2
PFDoA	5-12	2-3	7-12	4-5	1-4	2	9	3	9	4	3	2

BCC, back-calculated concentration; QC, quality control sample; PFHxA, perfluorohexanoic acid; HFPO-DA, ammonium perfluoro (2-methyl-3-oxa) hexanoate; PFHpA, perfluoroheptanoic acid; NaDONA, sodium dodecafluoro-3H-4.8-dioxanonanoate; PFBS, potassium perfluorobutanesulfonate; PFHxS, sodium perfluorohexanesulfonate; PFOA, perfluorooctanoic acid; PFNA, perfluorononanoic acid; PFOS, perfluorooctanesulfonic acid; PFDA, perfluorodecanoic acid; N-MeFOSAA, N-methyl perfluorooctanesulfonamidoacetic acid; PFUdA, perfluoroundecanoic acid; PFDoA, perfluorododecanoic acid.