Supplementary Files

Occurrence, Distribution, and Risk Assessment of Perfluoroalkyl Acids (PFAAs) in Muscle and Liver of Cattle in Xinjiang, China

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Table S1. The MS optimize parameters of 13 PFAAs and 2 internal standards.

Compounds	Parent ion (m/z)	Daughter ion (m/z)	Retention time (min)	Fragment (V)	Collision energy (V)	Internal standard
PFBA	213	169*/93	1.15	70/70	3/15	MPFOA
PFPeA	263	219*/113	1.35	70/70	5/15	MPFOA
PFHxA	313	269*/119	1.70	70/70	3/15	MPFOA
PFHpA	363	319*/169	2.44	70/70	5/10	MPFOA
PFOA	413	369*/168.9	3.91	70/70	4/9	MPFOA
PFNA	463	419*/219	5.67	70/70	5/10	MPFOA
PFDA	513	469*/269	6.87	70/70	5/15	MPFOA
PFUdA	563	519*/269	7.83	70/70	5/20	MPFOA
PFDoA	613	569*/169	8.69	70/70	4/24	MPFOA
PFTrDA	663	619*/169	9.47	70/70	5/25	MPFOA
PFBS	299	99*/80	2.04	70/70	30/40	MPFOS
PFHxS	399	90*/80	4.89	70/70	40/48	MPFOS
PFOS	499	99*/80	7.48	70/70	48/72	MPFOS
MPFOA	417	372*/172	3.91	70/70	4/9	--
MPFOS	503	99*/80	7.48	70/70	48/72	--

*Quantitative ion pair.

Table S2. Linear equation, correlation coefficient, LODs, LOQs, recovery, and RSDs of 13 PFAAs in beef muscle and beef liver.

Analyte	Beef muscle						Beef liver					
	Linear equation	R^2	LOD (ng/g)	LOQ (ng/g)	Recovery[a] (%, n=6)	RSD (%, n=6)	Linear equation	R^2	LOD (ng/g)	LOQ (ng/g)	Recovery[a] (%, n=6)	RSD (%, n=6)
MPFOA					90.4	3.2					81.5	4.1
MPFOS					82.3	3.7					78.6	3.3
PFBA	y=547.02x	0.9979	0.023	0.077	110.5	7.1	y=911.79x	0.9986	0.015	0.050	80.9	5.2
PFPeA	y=720.80x	0.9918	0.050	0.167	103.6	5.8	y=1437.07x	0.9959	0.027	0.090	88.2	4.7
PFHxA	y=940.20x	0.9982	0.061	0.203	100.1	6.5	y=2270.31x	0.9959	0.010	0.033	86.5	5.1
PFHpA	y=862.44x	0.9937	0.031	0.103	91.5	4.6	y=1928.18x	0.9972	0.030	0.100	91.6	4.3
PFOA	y=921.27x	0.9998	0.021	0.070	106.2	6.2	y=1844.85x	0.9984	0.017	0.057	85.4	4.1
PFNA	y=1259.96x	0.9975	0.019	0.063	115.4	7.3	y=1551.80x	0.9975	0.008	0.027	104.1	3.5
PFDA	y=1300.95x	0.9991	0.017	0.057	108.6	5.7	y=1651.67x	0.9992	0.014	0.047	94.3	3.0
PFUdA	y=1486.35x	0.9981	0.037	0.123	103.8	8.3	y=1850.06x	0.9985	0.004	0.013	101.8	6.2
PFDoA	y=1526.18x	0.9986	0.012	0.040	93.6	5.5	y=2898.38x	0.9983	0.007	0.023	84.2	4.5
PFTrDA	y=1260.73x	0.9964	0.012	0.040	73.8	8.9	y=1737.77x	0.9978	0.003	0.010	90.4	5.6
PFBS	y=301.25x	0.9914	0.040	0.133	75.3	9.4	y=540.40x	0.9953	0.013	0.043	100.6	5.7
PFHxS	y=201.77x	0.9951	0.061	0.203	84.7	7.8	y=318.15x	0.9978	0.036	0.120	110.0	4.4
PFOS	y=220.77x	0.9976	0.013	0.043	88.2	4.6	y=254.27x	0.9978	0.009	0.030	103.6	6.3

[a] The mean recovery at 0.02, 0.5, 1 ng/g spiked levels; R^2: correlation coefficient; LOD: the limits of detection; LOQ: the limits of quantification; RSD: relative standard deviation.