

## **Supplementary Materials**

### **Occurrence and Risk Assessment of Perfluoroalkyl Substances in Surface Water of Hefei City, Southeast China**

**Table S1.** The full name, abbreviation, and commercial sources of individual PFASs and internal standards

Full name	Abbreviation	Purity	Commercial sources
Perfluorobutyric acid	PFBA	HPLC grade	Alta Scientific Co, Ctd.
Perfluorovaleric acid	PFPA	HPLC grade	Alta Scientific Co, Ctd.
Perfluorohexanoic acid	PFHxA	HPLC grade	Alta Scientific Co, Ctd.
Perfluoroheptanoic acid	PFHpA	HPLC grade	Alta Scientific Co, Ctd.
Perfluorooctanoic acid	PFOA	HPLC grade	Alta Scientific Co, Ctd.
Perfluorononanoic acid	PFNA	HPLC grade	Alta Scientific Co, Ctd.
Perfluorodecanoic acid	PFDA	HPLC grade	Alta Scientific Co, Ctd.
Perfluorobutanesulfonic acid	PFBS	HPLC grade	Alta Scientific Co, Ctd.
Perfluorohexanesulfonic acid	PFHxS	HPLC grade	Alta Scientific Co, Ctd.
Perfluoroheptanesulfonic acid	PFHpS	HPLC grade	Alta Scientific Co, Ctd.
Perfluorooctanesulfonic acid	PFOS	HPLC grade	Alta Scientific Co, Ctd.
Perfluorohexanoic acid- $^{13}\text{C}_2$	PFHxA- $^{13}\text{C}_2$	HPLC grade	Alta Scientific Co, Ctd.
Perfluorooctanoic acid-1,2,3,4- $^{13}\text{C}_4$	PFOA- $^{13}\text{C}_4$	HPLC grade	Alta Scientific Co, Ctd.
Sodium Perfluorooctanesulfonate-1,2,3,4- $^{13}\text{C}_4$	PFOS- $^{13}\text{C}_4$	HPLC grade	Alta Scientific Co, Ctd.

**Table S2.** Specific geographic locations of sampling sites

Site	Longitude	Latitude	Site	Longitude	Latitude
W1	117.1129	31.7846	W12	117.4328	31.1596
W2	117.2588	31.5023	W13	117.1952	31.7107
W3	117.2689	31.6469	W14	117.3610	31.7496
W4	117.6754	31.6653	W15	117.3287	31.7628
W5	117.4352	32.0246	W16	117.2533	31.4367
W6	117.2477	31.8795	W17	117.3659	31.4768
W7	117.0771	31.8029	W18	117.3706	31.8068
W8	117.8566	31.7837	W19	117.5139	31.3558
W9	117.1168	31.0999	W20	117.7998	31.6602
W10	117.4238	31.7606	W21	118.7434	32.7174
W11	117.4480	31.7834	W22	117.2407	31.9265

**Table S3.** Structural information on the target and instrument parameter settings

Analytes	Abbreviation	Molecular Formula	Parent ion ( $m/z$ )	daughter ion ( $m/z$ )	Collision Energy
Perfluorobutyric acid	PFBA	C <sub>4</sub> HF <sub>7</sub> O <sub>2</sub>	213	169* 97	8 14
Perfluorovaleric acid	PFPA	C <sub>5</sub> HF <sub>9</sub> O <sub>2</sub>	263	219* 69	6 46
Perfluorohexanoic acid	PFHxA	C <sub>6</sub> HF <sub>11</sub> O <sub>2</sub>	313	269* 119	10 18
Perfluoroheptanoic acid	PFHpA	C <sub>7</sub> HF <sub>13</sub> O <sub>2</sub>	363	169* 119	14 22
Perfluorooctanoic acid	PFOA	C <sub>8</sub> HF <sub>15</sub> O <sub>2</sub>	413	169* 219	18 12
Perfluorononanoic acid	PFNA	C <sub>9</sub> HF <sub>17</sub> O <sub>2</sub>	463	219* 169	14 16
Perfluorodecanoic acid	PFDA	C <sub>10</sub> HF <sub>19</sub> O <sub>2</sub>	513	219* 269	15 15
Perfluorobutanesulfonic acid	PFBS	C <sub>4</sub> HF <sub>9</sub> O <sub>3</sub> S	299	80* 99	30 26
Perfluorohexanesulfonic acid	PFHxS	C <sub>6</sub> HF <sub>13</sub> O <sub>3</sub> S	399	80* 99	38 34
Perfluoroheptanesulfonic acid	PFHpS	C <sub>7</sub> HF <sub>15</sub> O <sub>3</sub> S	449	80* 99	38 34
Perfluorooctanesulfonic acid	PFOS	C <sub>8</sub> HF <sub>17</sub> O <sub>3</sub> S	499	80* 99	52 36
Perfluorohexanoic acid- <sup>13</sup> C <sub>2</sub>	PFHxA <sup>13</sup> C <sub>2</sub>	<sup>13</sup> C <sub>2</sub> C <sub>4</sub> HF <sub>11</sub> O <sub>2</sub>	315	270* 120	10 20
Perfluorooctanoic acid- 1,2,3,4- <sup>13</sup> C <sub>4</sub>	PFOA <sup>13</sup> C <sub>4</sub>	<sup>13</sup> C <sub>4</sub> C <sub>4</sub> HF <sub>15</sub> O <sub>2</sub>	417	169* 222	16 12
Sodium				80*	52
Perfluorooctanesulfonate- 1,2,3,4- <sup>13</sup> C <sub>4</sub>	PFOS <sup>13</sup> C <sub>4</sub>	<sup>13</sup> C <sub>4</sub> C <sub>4</sub> F <sub>17</sub> O <sub>3</sub> SNa	503	99	36

\*: iron for quantification

**Table S4.** Concentration range and detection rate of PFASs in surface water (ng/L)

Site	PEBA	PEPA	PFHxA	PFHnA	PEOA	PFNA	PEDA	PFBS	PFHxS	PFHnS	PFOS	$\Sigma_{11}$ PFASs
W1	6.18	4.72	10.22	2.82	28.60	2.90	1.37	102.20	0.07	ND	2.85	161.93
W2	3.72	4.71	9.89	5.05	16.00	2.78	0.61	2.65	1.47	2.10	38.70	87.68
W3	4.08	4.12	7.02	3.11	11.30	6.94	2.71	14.10	0.53	0.06	10.40	64.37
W4	6.53	3.00	6.53	4.32	13.50	3.22	0.52	7.27	1.08	0.09	3.98	50.04
W5	24.00	4.51	7.99	3.32	14.40	1.95	0.66	5.13	0.44	0.02	2.46	64.88
W6	4.28	5.81	8.17	2.21	32.00	2.47	1.07	8.98	0.11	0.23	5.06	70.38
W7	15.80	12.40	11.30	3.92	10.30	4.41	0.95	20.90	ND	ND	1.15	81.13
W8	2.00	0.81	1.63	1.19	5.29	1.94	ND	0.47	ND	ND	0.56	13.89
W9	28.10	26.00	18.40	6.50	8.61	3.85	1.39	77.00	0.42	ND	2.85	173.12
W10	33.10	6.19	8.80	2.76	13.20	2.51	0.98	10.60	0.12	0.12	2.98	81.36
W11	6.19	3.94	7.12	3.26	13.60	3.16	0.83	9.46	0.27	0.20	15.20	63.23
W12	99.20	193.80	183.40	7.96	53.20	3.90	ND	3.44	ND	ND	0.60	545.50
W13	5.63	3.07	8.16	1.91	7.95	1.98	0.98	20.10	0.61	0.39	8.88	59.63
W14	3.04	1.37	3.35	1.50	7.46	1.97	0.35	6.04	0.13	0.06	2.80	28.05
W15	2.64	1.09	2.63	1.29	6.72	1.68	ND	7.14	0.17	0.03	1.93	25.29
W16	4.21	2.18	4.53	2.45	25.2	2.91	0.88	2.97	ND	ND	0.62	45.95
W17	1.97	1.08	1.93	1.57	7.19	3.65	1.12	0.80	0.13	ND	0.89	20.33
W18	15.8	1.44	3.28	1.24	8.21	1.80	0.80	2.91	0.24	ND	2.43	38.15
W19	2.14	1.30	2.77	1.92	7.75	3.00	0.69	2.38	0.058	0.10	0.93	23.04
W20	3.86	2.75	6.48	3.18	13.30	3.40	0.87	3.92	0.019	ND	0.59	38.37
W21	1.06	0.26	3.10	0.78	3.78	1.07	0.38	0.99	0.23	ND	1.05	12.70
W22	1.62	0.45	1.78	1.03	4.41	1.46	0.38	1.30	0.25	ND	0.36	13.04
Detection	100	100	100	100	100	100	86.4	100	81.8	50	100	—

ND: Not detected or lower than the LOQ.

**Table S5.** Risk quotients for PFOA, PFOS, PFNA, PFHxA and PFDA at each site

Site	RQ( $\times 10^{-4}$ )				
	PFOA	PFOS	PFNA	PFHxA	PFDA
W1	0.50	1.14	0.29	1.05	1.24
W2	0.28	15.48	0.28	1.02	0.55
W3	0.20	4.16	0.69	0.72	2.46
W4	0.24	1.59	0.32	0.67	0.47
W5	0.25	0.98	0.20	0.82	0.60
W6	0.56	2.02	0.25	0.84	0.97
W7	0.18	0.46	0.44	1.16	0.86
W8	0.09	0.22	0.19	0.17	0.00
W9	0.15	1.14	0.39	1.90	1.26
W10	0.23	1.19	0.25	0.91	0.89
W11	0.24	6.08	0.32	0.73	0.75
W12	0.93	0.24	0.39	18.91	0.00
W13	0.14	3.55	0.20	0.84	0.89
W14	0.13	1.12	0.20	0.35	0.32
W15	0.12	0.77	0.17	0.27	0.00
W16	0.44	0.25	0.29	0.47	0.80
W17	0.13	0.35	0.37	0.20	1.02
W18	0.14	0.97	0.18	0.34	0.73
W19	0.14	0.38	0.30	0.29	0.63
W20	0.23	0.24	0.34	0.67	0.79
W21	0.07	0.42	0.11	0.32	0.35
W22	0.08	0.14	0.15	0.18	0.35