

Supplementary Information

for

Characteristics, source apportionment and health risk assessment of perfluoroalkyl acids in typical drinking water sources of eastern China

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Table S1 Basic information of sampling sites

Category	Site symbol	Location	Category	Site symbol	Location
ER-SNWDP lakes-reservoirs	S01	116.74°E, 35.08 °N	Yellow River reservoir	S13	117.90°E, 37.21°N
	S02	117.28°E, 34.65 °N		S14	118.31°E,37.33°N
	S03	116.29°E, 35.95°N		S15	118.69°E,37.40°N
	S04	117.31°E, 36.87°N		S16	118.68°E,37.47°N
	S05	116.80°E, 34.65°N		S17	118.07°E,37.40°N
	S06	116.98°E, 36.77°N		S18	115.36°E,35.25°N
Yellow River reservoir	S07	117.15°E, 37.47°N	local reservoir	S19	115.55°E,35.06°N
	S08	117.20°E, 37.04°N		S20	116.47°E,37.32°N
	S09	120.05°E,36.02°N		S21	116.20°E, 37.30°N
	S10	120.25°E,36.35°N		S22	116.33°E,37.42°N
	S11	119.08°E,36.62°N		S23	116.96°E,36.49°N
	S12	119.40°E,36.50°N		S24	118.10°E, 35.68°N

Table S2 Basic water quality parameters of the samples taken

Site symbol	pH		Dissolved oxygen (mg·L ⁻¹)		Ammonia nitrogen (mg·L ⁻¹)		Chloride (mg·L ⁻¹)		Sulfate (mg·L ⁻¹)		COD (mg·L ⁻¹)	
	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry
S01	8.3	8.6	7.3	10.0	0.22	0.29	405	153	336	214	29	36
S02	8.6	8.8	7.8	9.8	0.20	0.17	632	106	255	172	27	26
S03	7.8	8.2	5.3	12.3	0.29	0.10	132	146	146	222	11	16
S04	8.2	8.2	10.4	9.3	0.07	0.03	111	107	179	180	14	16
S05	8.3	8.2	8.2	10.3	0.05	0.05	100	73.2	174	128	11	11
S06	8.3	8.2	9.1	10.3	<0.03	<0.03	81.5	57.1	146	118	10	11
S07	8.4	8.3	8.2	9.3	<0.03	<0.03	134	121	193	188	12	10
S08	8.3	8.4	8.6	9.9	0.03	0.04	81.4	55.0	148	113	19	10
S09	8.2	8.3	10.0	12.2	0.08	0.10	48	52	41	63	15	21
S10	7.7	8.2	9.6	12.9	0.08	0.04	126	164	128	150	12	20
S11	7.8	8.2	9.1	12.8	0.13	0.15	85	91.4	108	119	11	14
S12	7.9	8.3	11.8	13.1	0.13	0.16	156	152	100	102	14	20
S13	7.6	8.3	10.0	13.2	0.14	0.16	99	92.5	100	150	8	12
S14	7.8	8.2	8.8	12.4	0.06	0.08	170	89	153	129	10	14
S15	7.3	8.2	8.6	12.4	0.05	0.05	96	208	164	138	5	12
S16	7.4	8.1	7.9	10.1	0.06	0.07	115	266	156	182	14	14
S17	7.9	8.2	9.7	11.6	0.05	0.07	117	84.6	149	122	12	18
S18	7.7	7.5	10.5	12.6	0.07	0.07	102	82.8	128	126	12	12
S19	7.7	8.2	10.5	11.8	0.07	0.06	172	156	154	180	8	20
S20	7.3	8.4	9.0	13.2	0.05	0.07	42	91.4	207	168	10	14
S21	7.3	8.2	8.7	13.3	0.05	0.09	98	200	240	314	14	15

S22	7.3	8.4	9.0	14.1	0.05	0.09	7.80	90.7	131	140	6	14
S23	8.3	8.1	8.9	9.1	0.12	<0.03	15.3	17.6	76	84	10	9
S24	7.8	8.9	10.0	12.0	0.08	0.07	20	21	89	96	11	12

Note: Wet represents the wet season. Dry represents the dry season.

Table S3 Mobile phase gradient for instrumental analysis

Time/mi	%A	%B
Initial	65	35
1	50	50
6	30	70
7	10	90
8.5	10	90
8.51	65	35
10	65	35

Table S4 Mass spectrometric detection conditions of 17 target compounds

Target compounds	Retention time/min	Ion pair	Cone voltage/V	Collision energy/eV
PFBA	3.10	213/125	14	12
		213/169*	14	10
PFPeA	4.71	263/141	14	10
		263/219*	14	10
PFHxA	6.04	313/119	14	20
		313/269*	14	10
PFHpA	7.34	363/169	14	18
		363/319*	14	10
PFOA	8.54	413/169	14	18
		413/369*	14	10
PFNA	9.47	463/169	16	20
		463/419*	16	10
PFDA	9.91	513/169	16	26
		513/469*	16	10
PFUnDA	10.19	563/169	16	26
		563/519*	16	11
PFDoDA	10.43	613/169	16	28
		613/569*	16	12
PFTrDA	10.67	663/169	16	32
		663/619*	16	12
PFTeDA	10.94	713/169	16	34
		713/669*	16	12
PFHxDA	10.07	813/169	30	34
		813/769*	30	12
PFoDA	10.31	913/169	20	34
		913/869*	20	15
PFDS	10.19	599/80	70	50
		599/99*	70	34
PFOS	9.55	499/80	60	32
		499/99*	60	30
PFHxS	7.62	399/80	60	32
		399/99*	60	30
PFBS	5.13	299/80	45	30
		299/99*	45	28

Note: * represents quantitative ion.

Table S5 Detection frequency, recovery, ranges, average and median concentrations of PFAAs for lakes and reservoirs in Shandong Province of eastern China in the wet season and dry season

Target compounds	The wet season				The dry season				MDL (ng·L ⁻¹)
	Range (ng·L ⁻¹)	Mean (ng·L ⁻¹)	Median (ng·L ⁻¹)	DF (%)	Range (ng·L ⁻¹)	Mean (ng·L ⁻¹)	Median (ng·L ⁻¹)	DF (%)	
PFBA	ND	/	/	0/24 (0)	ND	/	/	0/24 (0)	1.0
PFPeA	ND	/	/	0/24 (0)	ND	/	/	0/24 (0)	1.0
PFHxA	ND~18.0	6.5	5.0	8/24 (33.3%)	ND~2.1	1.4	1.4	11/24 (45.8%)	0.5
PFHpA	ND~9.0	3.6	3.0	10/24 (41.7%)	ND~2.4	1.0	0.9	15/24 (62.5%)	0.3
PFOA	0.9~92.7	21.9	6.9	24/24 (100%)	1.9~37.6	13.2	8.8	24/24 (100%)	0.5
PFNA	ND~2.1	1.0	1.0	13/24 (54.2%)	ND~0.95	0.3	0.23	17/24 (70.8%)	0.1
PFDA	ND	/	/	0/24 (0)	ND	/	/	0/24 (0)	0.5
PFUnDA	ND	/	/	0/24 (0)	ND	/	/	0/24 (0)	1.0
PFDoDA	ND	/	/	0/24 (0)	ND	/	/	0/24 (0)	1.0
PFTTrDA	ND	/	/	0/24 (0)	ND	/	/	0/24 (0)	1.0
PFTeDA	ND	/	/	0/24 (0)	ND	/	/	0/24 (0)	2.0
PFHxDA	ND	/	/	0/24 (0)	ND	/	/	0/24 (0)	1.0
PFODA	ND	/	/	0/24 (0)	ND	/	/	0/24 (0)	1.0

1.	PFDS	ND	/	/	(0) 0/24 (0)	ND	/	/	(0) 0/24 (0)	1.0	Note: DF
=	PFOS	ND~3.0	2.2	2.0	5/24 (20.8%)	ND~1.2	0.8	0.7	8/24 (33.3%)	0.5	
	PFHxS	ND~4.0	2.0	2.0	10/24 (41.7%)	ND~1.7	0.6	0.5	10/24 (41.7%)	0.3	
	PFBS	ND~4.0	2.8	2.5	8/24 (33.3%)	ND~2.8	0.75	0.75	18/24 (75%)	0.3	

detection frequency; SD = standard deviation; ND = not detected.

2. The mean and median values were calculated based on the concentration detected by individual PFAA.

Table S6 Mean body weight (BW), the quantity of drinking water intake (DWI), and the acceptable daily intake of PFAAs values (ADI) for different age/gender groups in China

Age group	Gender	BW/kg ¹	DWI/L·d ^{-1 2}	ADI/ng·kg ⁻¹ ·d ⁻¹						
				PFOA ³	PFNA ⁴	PFOS ⁵	PFHpA ⁴	PFHxA ⁴	PFHxS ⁴	PFBS ⁴
3~6	male	19.63	1.08	200	4150	150	100000	100000	5000	500000
	female	18.65	1.08	200	4150	150	100000	100000	5000	500000
7~11	male	33.84	1.24	200	4150	150	100000	100000	5000	500000
	female	31.94	1.24	200	4150	150	100000	100000	5000	500000
12~16	male	55.16	1.73	200	4150	150	100000	100000	5000	500000
	female	49.44	1.73	200	4150	150	100000	100000	5000	500000
17~19	male	63.43	2.26	200	4150	150	100000	100000	5000	500000
	female	52.67	2.26	200	4150	150	100000	100000	5000	500000
20~24	male	67.20	2.81	200	4150	150	100000	100000	5000	500000
	female	53.80	2.81	200	4150	150	100000	100000	5000	500000
25~59	male	70.77	2.81	200	4150	150	100000	100000	5000	500000
	female	58.37	2.81	200	4150	150	100000	100000	5000	500000
>60	male	67.10	2.81	200	4150	150	100000	100000	5000	500000
	female	59.45	2.81	200	4150	150	100000	100000	5000	500000

Table S7 Total variances in PCA of PFAAs for lakes and reservoirs in Shandong Province of eastern China in the wet season

Component	Initial eigenvalue			Quadratic sum of extracted loading			Quadratic sum of rotated loading		
	Aggregate	Variance percent	Cumulative (%)	Aggregate	Variance percent	Cumulative (%)	Aggregate	Variance percent	Cumulative (%)
1	4.754	67.921	67.921	4.754	67.921	67.921	4.006	57.223	57.223
2	1.083	15.464	83.386	1.083	15.464	83.386	1.831	26.163	83.386

Table S8 Rotated factor loading matrix in PCA of PFAAs in lakes and reservoirs from the lower reaches of the Yellow River in the wet season and dry season

PFAAs	Wet season		Dry season		
	Factor 1	Factor 2	Factor 1	Factor 2	Factor 3
PFOA	0.882	-0.148	0.104	0.104	0.379
PFNA	0.846	0.285	0.157	0.251	-0.051
PFOS	0.551	0.720	-0.242	0.899	0.005
PFHxA	0.847	0.360	0.324	-0.191	0.034
PFHxS	0.056	0.908	-0.112	-0.019	0.795
PFHpA	0.892	0.382	0.257	0.030	-0.016
PFBS	0.832	0.332	0.380	-0.309	-0.259

Table S9 Total variances in PCA of PFAAs for lakes and reservoirs in Shandong Province of eastern China in the dry season

Component	Initial eigenvalue			Quadratic sum of extracted loading			Quadratic sum of rotated loading		
	Aggregate	Variance percent	Cumulative (%)	Aggregate	Variance percent	Cumulative (%)	Aggregate	Variance percent	Cumulative (%)
1	3.971	56.731	56.731	3.971	56.731	56.731	3.418	48.835	48.835
2	1.236	17.653	74.384	1.236	17.653	74.384	1.343	19.190	68.025
3	0.817	11.672	86.056	0.817	11.672	86.056	1.262	18.031	86.056

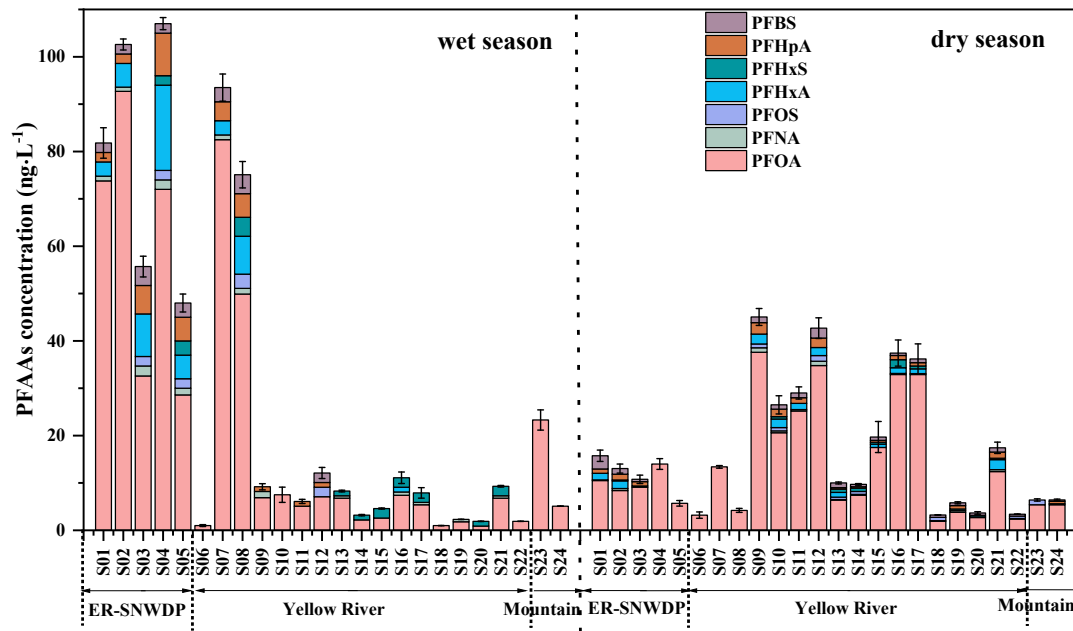


Fig. S1 Concentration profiles of PFAAs in the 24 lakes and reservoirs for the wet season and dry season

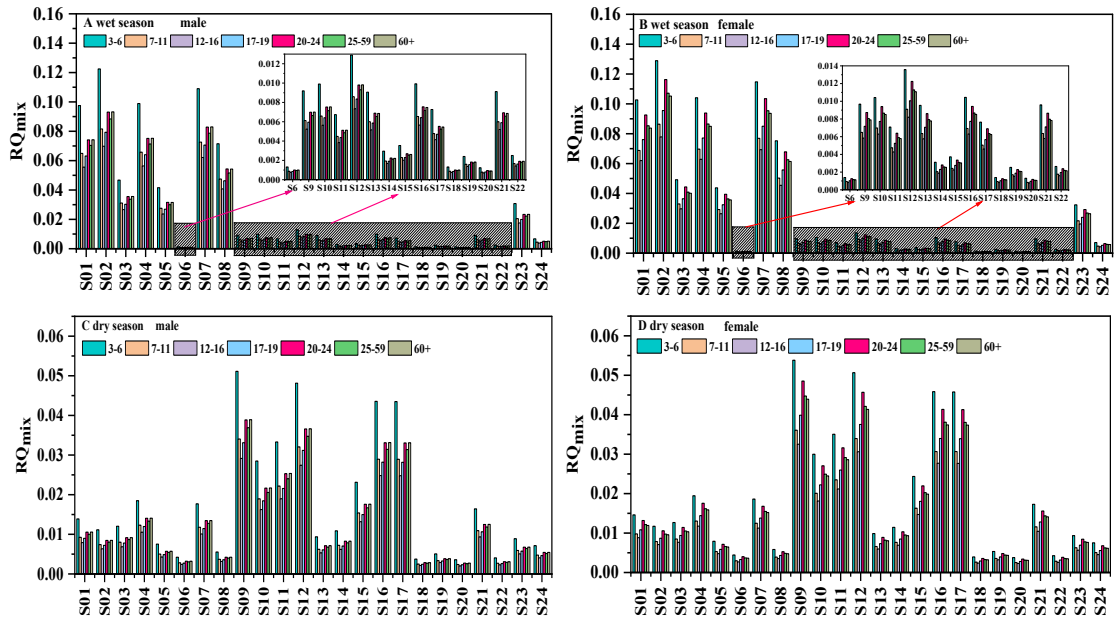


Fig. S2 RQ_{mix} values for Σ PFAs related to drinking water intake for male (A) and female (B) in the wet season and male (C) and female (D) in the dry season for all sampling sites

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