

Supporting information for

Spatial distribution and source apportionment of PFASs in surface sediments from five lake regions, China

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Number of tables: 3

Number of figures: 2

Number of pages: 8

Supporting information legends

Table S1 | Abbreviations, mass transitions, retention times (min) for the studied perfluoroalkyl substances (PFASs)

Table S2 | Geographic and limnological features of forty-eight lakes and two reservoirs studied

Table S3 | Limits of detection (ng/mL), limits of quantitation (ng/mL), blank spike recoveries (%), n=5) and matrix spike recoveries (%), n=5) for PFASs (n indicates the number of samples analyzed; mean \pm SD) ^a

Figure S1 | A map plotting for forty-eight lakes and two reservoirs studied. (We created the map using the ArcGIS 9.2 software for windows 2000/XP/VISTA/7 and the Microsoft Office 2010 software for windows 2003/XP/VISTA/7.)

Figure S2 | Concentrations (ng/g dw) of PFASs in surface sediments from China, Japan, Austria, Germany, Australia, the USA and Canada (including sample size ≥ 1 ; No bar: no corresponding values) ⁸⁻¹⁵. (We created the map using the Microsoft Office 2010 software for windows 2003/XP/VISTA/7.)

Table S1 | Abbreviations, mass transitions, retention times (min) for the studied perfluoroalkyl substances (PFASs)

Analyte	Acronym	Precursor/product ion	Retention time	Quantification by internal standard
Target analytes				
Perfluorobutyric acid	PFBA	212.9/168.9	1.68	¹³ C ₄ -PFBA
Perfluoropentanoic acid	PFPeA	262.9/218.9, 262.9/69.0	2.19	¹³ C ₄ -PFBA
Perfluorohexanoic acid	PFHxA	312.9/268.9, 312.9/119.1	2.78	¹³ C ₂ -PFHxA
Perfluoroheptanoic acid	PFHpA	362.9/318.9, 362.9/168.9	3.41	¹³ C ₂ -PFHxA
Perfluorooctanoate acid	PFOA	412.9/368.9, 412.9/169.0	4.00	¹³ C ₄ -PFOA
Perfluorononanoic acid	PFNA	462.9/418.9, 462.9/218.9	4.53	¹³ C ₅ -PFNA
Perfluorodecanoic acid	PFDA	512.9/468.9, 512.9/268.9	5.03	¹³ C ₂ -PFDA
Perfluoroundecanoic acid	PFUnDA	562.9/518.8, 562.9/268.8	5.48	¹³ C ₂ -PFUnDA
Perfluorododecanoic acid	PFDoDA	612.9/568.9, 612.9/318.8	5.83	¹³ C ₂ -PFDoDA
Perfluorotridecanoic acid	PFTTrDA	662.9/618.9, 662.9/368.9	6.15	¹³ C ₂ -PFDoDA
Perfluorotetradecanoic acid	PFTeDA	712.9/668.9, 712.9/368.9	6.42	¹³ C ₂ -PFDoDA
Perfluorohexadecanoic acid	PFHxDA	812.9/768.9, 812.9/468.9	6.85	¹³ C ₂ -PFDoDA
Perfluorooctadecanoic acid	PFOcDA	912.9/869.1, 912.9/568.9	7.22	¹³ C ₂ -PFDoDA
Perfluorobutane sulfonic acid	PFBS	298.9/99, 298.9/79.9	2.29	¹⁸ O ₂ -PFHxS
Perfluorohexane sulfonic acid	PFHxS	398.9/99, 398.8/79.9	3.44	¹⁸ O ₂ -PFHxS
Perfluorooctane sulfonic acid	PFOS	498.9/99, 498.9/79.9	4.56	¹³ C ₄ -PFOS
Perfluorodecane sulfonic acid	PFDS	598.9/99, 598.9/79.9	5.46	¹³ C ₄ -PFOS
Internal standards				
Perfluoro-n-[1,2,3,4- ¹³ C ₄] butanoic acid	¹³ C ₄ -PFBA	216.9/171.9	1.67	¹³ C ₈ -PFOA
Perfluoro-n-[1,2- ¹³ C ₂] hexanoic acid	¹³ C ₂ -PFHxA	314.9/269.9	2.77	¹³ C ₈ -PFOA
Perfluoro-n-[1,2,3,4- ¹³ C ₄] octanoic acid	¹³ C ₄ -PFOA	416.9/371.9	3.99	¹³ C ₈ -PFOA
Perfluoro-n-[1,2,3,4,5- ¹³ C ₅] nonanoic acid	¹³ C ₅ -PFNA	467.9/422.9	4.52	¹³ C ₈ -PFOA
Perfluoro-n-[1,2- ¹³ C ₂] decanoic acid	¹³ C ₂ -PFDA	514.9/469.9	5.02	¹³ C ₈ -PFOA
Perfluoro-n-[1,2- ¹³ C ₂] undecanoic acid	¹³ C ₂ -PFUnDA	564.9/519.8	5.46	¹³ C ₈ -PFOA
Perfluoro-n-[1,2- ¹³ C ₂] dodecanoic acid	¹³ C ₂ -PFDoDA	614.9/569.9	5.82	¹³ C ₈ -PFOA
Perfluoro-1-hexane [¹⁸ O ₂] sulfonate	¹⁸ O ₂ -PFHxS	402.9/103.0	3.43	¹³ C ₈ -PFOS
Perfluoro-1- [1,2,3,4- ¹³ C ₄] octanesulfonate	¹³ C ₄ -PFOS	502.9/99.1	4.57	¹³ C ₈ -PFOS

Table S2 | Geographic and limnological features of forty-eight lakes and two reservoirs studied

Lake region	Lake	Serial number	Sampling time	Sample site	Position	Lake area (km ²)	Mean depth (m)	Catchment area (km ²)
East Plain Region	Lake Wabu ¹	1	2012.04	Anhui Province	116°48′~117°01′E 32°23′~32°33′N	163	2.42	800
	Lake Longgan ¹	2	2012.06	Anhui Province	115°19′~116°17′E 29°52′~30°05′N	316	3.78	5,511
	Lake Shengjin ¹	3	2012.07	Anhui Province	116°58′~117°14′E 30°15′~30°28′N	78.5	1.26	1,554
	Lake Xiangjian ¹	4	2011.10	Anhui Province	117°15′~117°45′E 33°06′~33°12′N	45.0	0.93	-
	Lake Chengdong ¹	5	2012.04	Anhui Province	116°18′~116°28′E 32°12′~32°22′N	120	1.50	2,128
	Lake Chengxi ¹	6	2012.04	Anhui Province	116°01′~116°18′E 32°11′~32°33′N	199	2.70	1,750
	Lake Huayuan ¹	7	2011.10	Anhui Province	117°45′~117°53′E 32°55′~33°02′N	34.0	1.35	875
	Lake Baidang ¹	8	2012.07	Anhui Province	117°19′~117°27′E 30°47′~30°51′N	39.7	3.06	775
	Lake Bohu ¹	9	2012.06	Anhui Province	116°19′~116°33′E 30°04′~30°15′N	180	4.41	-
	Lake Wuchang ¹	10	2012.06	Anhui Province	116°36′~116°53′E 30°14′~30°20′N	101	3.43	1,084
	Lake Huangdahu ¹	11	2012.06	Anhui Province	116°14′~116°33′E 29°56′~30°08′N	299	3.94	-
	Lake Tuohu ¹	12	2011.10	Anhui Province	117°45′~117°51′E 33°09′~33°17′N	40.0	1.20	-
	Lake Nvshan ¹	13	2011.10	Anhui Province	117°58′~118°14′E 32°50′~33°02′N	105	1.71	4,215
	Lake Chaohu ¹	14	2011.12	Anhui Province	117°16′~117°05′E 31°25′~31°43′N	770	2.69	9,258
	Lake Luoma ¹	15	2013.06	Jiangsu Province	118°04′~118°18′E 34°00′~34°14′N	260	3.30	51,215
	Lake Cheng ¹	16	2013.07	Jiangsu Province	120°48′~120°52′E 31°10′~31°14′N	45.0	1.83	-
	Lake Yuandang ¹	17	2013.07	Jiangsu Province	120°51′~120°54′E 31°03′~31°05′N	12.9	1.38	-
	Lake Yaohu ¹	18	2013.08	Jiangsu Province	119°30′~119°40′E 31°30′~31°40′N	89.0	1.10	-
	Lake Gucheng ¹	19	2013.08	Jiangsu Province	118°53′~118°57′E 31°14′~31°18′N	24.5	1.56	248
	Lake Gehu ¹	20	2013.08	Jiangsu Province	119°44′~119°53′E 31°29′~31°42′N	147	1.19	-
	Lake Yangcheng ¹	21	2013.07	Jiangsu Province	120°39′~120°51′E 31°21′~31°30′N	119	1.40	-
	Lake Sanjiu ¹	22	2013.08	Jiangsu Province	119°48′E 31°22′N	23.2	1.85	-
	Lake Shijiu ¹	23	2013.08	Jiangsu Province	118°46′~118°56′E 31°23′~31°33′N	210	4.08	18,600
	Lake Gaoyou ¹	24	2013.06	Jiangsu Province	119°06′~119°25′E 32°42′~33°04′N	675	1.44	158,148
	Lake Nansi ¹	25	2013.06	Jiangsu Province	116°34′~117°21′E 34°27′~35°20′N	1,098	1.46	30,453
	Lake Shaobo ¹	26	2013.06	Jiangsu Province	119°23′~119°30′E 32°30′~32°40′N	77.0	1.10	-
	Lake Hongze ¹	27	2013.06	Jiangsu Province	118°10′~118°52′E 33°06′~33°40′N	1,577	1.77	156,000
	Lake Kuncheng ¹	28	2013.07	Jiangsu Province	120°43′~120°46′E 31°33′~31°36′N	18.0	1.78	-
	Lake Baima ¹	29	2013.06	Jiangsu Province	119°03′~119°11′E 33°09′~33°19′N	108	0.97	950
Mengxin Plateau Lake Region	Lake Bositeng ¹	30	2011.10	Xinjiang Uygur Autonomous Region	86°41′~87°27′E 41°49′~42°08′N	992	8.08	27,000
	Lake Wulungu ¹	31	2011.10	Xinjiang Uygur Autonomous Region	87°02′~87°35′E 47°02′~47°25′N	753	8.00	32,000
Tibetan Plateau Lake Region	Lake Jili ¹	32	2011.10	Xinjiang Uygur Autonomous Region	87°20′~87°32′E 46°51′~47°00′N	174	9.90	-
	Lake Hulun ¹	33	2011.10	Inner Mongolia Autonomous Region	116°58′~117°48′E 48°30′~49°20′N	2,339	5.92	37,214
Tibetan Plateau Lake Region	Lake Wuliangsu ¹	34	2011.10	Inner Mongolia Autonomous Region	108°43′~108°57′E 40°47′~41°03′N	233	1.12	11,800
	Lake Qinghai ¹	35	2012.07	Qinghai Province	99°36′~100°47′E 36°32′~37°15′N	4,340	17.9	29,661
	Lake Basongcuo ²	36	2012.07	Tibet Autonomous Region	93°57′E 30°01′N	27.0	120 (Max.)	-
	Lake Yamdrok ¹	37	2012.07	Tibet Autonomous Region	90°21′~91°05′E 28°16′~29°11′N	638	20.0~40.0	5,422
Yungui Plateau Lake Region	Lake Namucuo ¹	38	2012.07	Tibet Autonomous Region	90°16′~91°03′E 30°30′~30°56′N	1,962	-	8,649
	Lake Yihai ^{3,4}	39	2010.08	Sichuan Province	102°14′E 28°44′N	1.00	9.80	-
	Daqiao Reservoir ⁵	40	2010.08	Sichuan Province	102°12′E 28°41′N	23.5	-	796
	Lake Qionghai ¹	41	2010.08	Sichuan Province	102°16′~102°21′E 27°47′~27°52′N	31.0	10.3	109
	Lake Mahu ¹	42	2010.08	Sichuan Province	103°47′~103°48′E 28°23′~28°26′N	7.30	65.7	97
	Lake Shudu ⁶	43	2010.06	Yunnan Province	99°57′E 27°55′N	1.70	7.80 (Max.)	14
	Lake Qilu ¹	44	2010.07	Yunnan Province	102°43′~102°49′E 24°08′~24°13′N	36.9	4.03	341
	Lake Chenghai ¹	45	2010.06	Yunnan Province	100°38′~100°41′E 26°27′~26°38′N	77.2	25.7	229
Northeast Plain Lake Region	Lake Lugu ¹	46	2010.06	Yunnan Province	100°45′~100°50′E 27°41′~27°45′N	48.5	40.3	171
	Lake Wudalianchi ¹	47	2012.07	Heilongjiang Province	126°06′~126°15′E 48°40′~48°47′N	16.4	1.00-12.00	-
	Lake Xingkai ¹	48	2012.07	Heilongjiang Province	131°58′~132°51′E 44°32′~45°21′N	1,080	6.28	56,000
	Dahuofang Reservoir ⁷	49	2012.07	Liaoning Province	120°20′~125°15′E 41°31′~42°15′N	22.0-91.2	-	5,437
Lake Jingbo ¹	50	2012.07	Heilongjiang Province	128°37′~129°03′E 43°46′~44°03′N	91.5	12.9	11,820	

Table S3 | Limits of detection (ng/mL), limits of quantitation (ng/mL), blank spike recoveries (% , n=5) and matrix spike recoveries (% , n=5) for PFASs (n indicates the number of samples analyzed; mean \pm SD) ^a

Acronym	Limits of detection	Limits of quantitation	Blank spike recoveries	Matrix spike recoveries	
				2 ng/mL	20 ng/mL
Target analytes					
PFBA	0.01	0.05	104 \pm 5	88 \pm 9	96 \pm 7
PFPeA	0.01	0.03	101 \pm 4	87 \pm 12	95 \pm 9
PFHxA	0.01	0.04	97 \pm 3	92 \pm 8	104 \pm 6
PFHpA	0.02	0.06	102 \pm 5	109 \pm 9	98 \pm 7
PFOA	0.02	0.05	96 \pm 4	114 \pm 8	102 \pm 6
PFNA	0.02	0.06	112 \pm 5	109 \pm 10	97 \pm 7
PFDA	0.02	0.05	98 \pm 9	91 \pm 13	95 \pm 10
PFUnDA	0.02	0.08	102 \pm 6	111 \pm 10	115 \pm 8
PFDoDA	0.01	0.03	99 \pm 4	91 \pm 10	105 \pm 7
PFTTrDA	0.01	0.05	96 \pm 7	88 \pm 12	108 \pm 9
PFTeDA	0.01	0.03	92 \pm 9	82 \pm 14	90 \pm 11
PFHxDA	0.06	0.20	89 \pm 8	77 \pm 13	84 \pm 11
PFOcDA	0.11	0.39	77 \pm 10	69 \pm 15	75 \pm 13
PFBS	0.02	0.06	98 \pm 3	90 \pm 7	102 \pm 8
PFHxS	0.01	0.04	99 \pm 4	109 \pm 9	93 \pm 6
PFOS	0.01	0.04	101 \pm 4	94 \pm 9	97 \pm 7
PFDS	0.01	0.03	96 \pm 5	92 \pm 8	90 \pm 8
Internal standards					
¹³ C ₄ -PFBA				93 \pm 9	
¹³ C ₂ -PFHxA				92 \pm 7	
¹³ C ₄ -PFOA				90 \pm 4	
¹³ C ₅ -PFNA				87 \pm 8	
¹³ C ₂ -PFDA				85 \pm 5	
¹³ C ₂ -PFUnDA				89 \pm 7	
¹³ C ₂ -PFDoDA				83 \pm 9	
¹⁸ O ₂ -PFHxS				90 \pm 7	
¹³ C ₄ -PFOS				92 \pm 6	

^a The spike recoveries of PFASs were calculated using the equation: spike recovery = $(C_{\text{sample} + \text{spiked}} - C_{\text{sample}}) / C_{\text{spiked}} \times 100\%$, where $C_{\text{sample} + \text{spiked}}$ is the concentration of PFASs in a spiked sample, C_{sample} is the concentration of PFASs in the sample (same as above without spiked target compounds), C_{spiked} is the concentration of the spiked target compound. The recoveries of the stable isotope-labeled internal standards were calculated by the ratio of concentrations in the samples compared with those in the standard solutions.



Figure S1 | A map plotting of forty-eight lakes and two reservoirs studied. (We created the map using the ArcGIS 9.2 software for windows 2000/XP/VISTA/7 and the Microsoft Office 2010 software for windows 2003/XP/VISTA/7.)

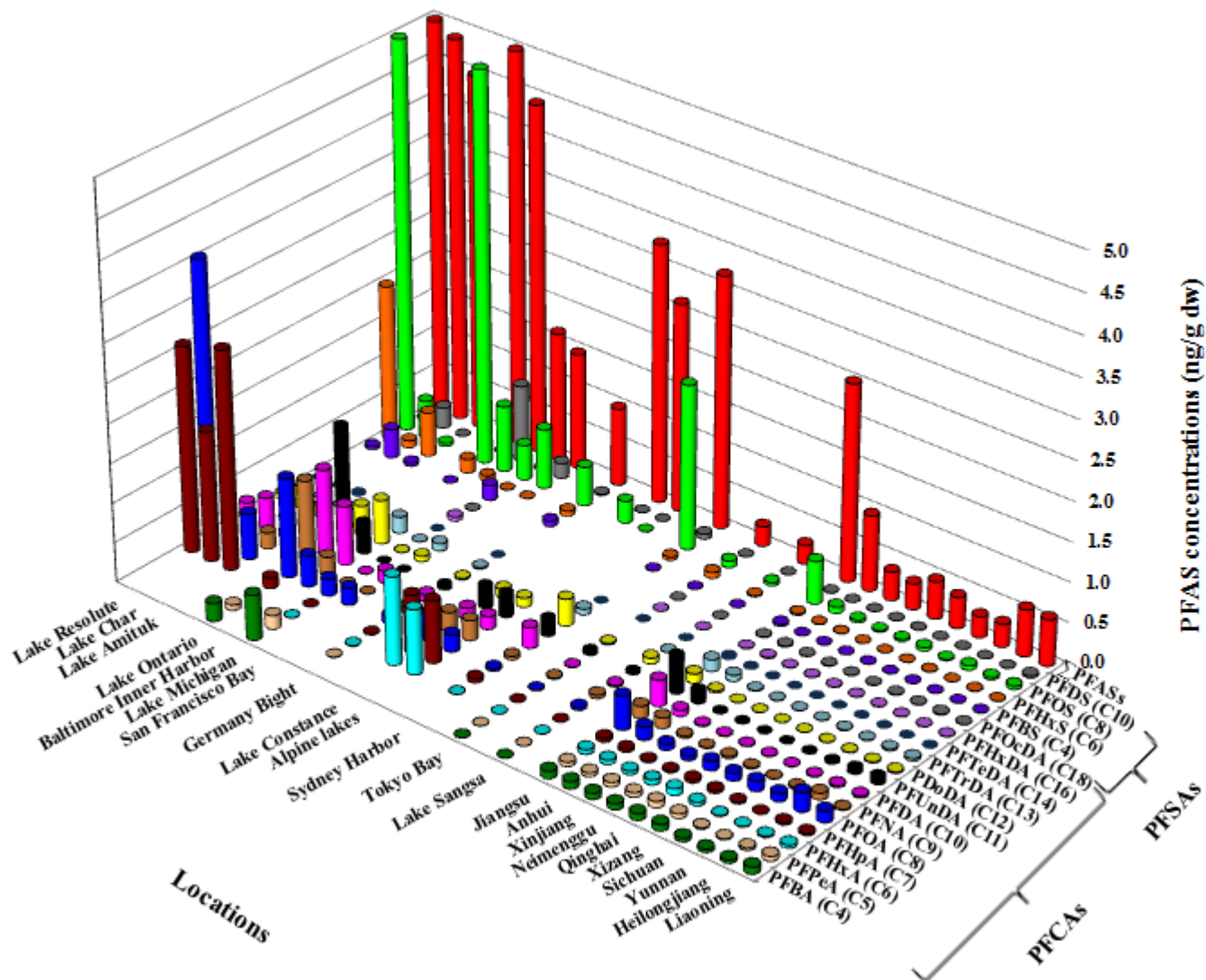


Figure S2 | Concentrations (ng/g dw) of PFASs in surface sediments from China, Japan, Austria, Germany, Australia, the USA and Canada (including sample size ≥ 1 ; No bar: no corresponding values)⁸⁻¹⁵. (We created the map using the Microsoft Office 2010 software for windows 2003/XP/VISTA/7.)

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