Supplementary Materials

Occurrence, sources and ecological risk assessment of per- and polyfluoroalkyl substances (PFASs) in water and sediment from urban rivers in Dhaka, Bangladesh

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Supplementary Table 1. Analytes, acronyms, supplier, purity, retention time, MS/MS transition, and corresponding internal standards

Classification	Compound name	Acronym	Supplier of standard and its purity	Retention time (min)	MS/MS transition (m/z)	Corresponding IS
PFCAs (perfluoroalkyl carboxylic acids)	Perfluorobutanoate	PFBA	PFC-MXA (Mix) Wellington Laboratories, 98%	6.17	212.7 → 168.7	[^{13}C4]PFBA
	Perfluoropentanoate	PFPeA		13.06	262.7 → 218.7	[^{13}C2]PFHxA
	Perfluorohexanoate	PFHxA		14.11	312.7 → 268.7	[^{13}C2]PFHxA
	Perfluoroheptanoate	PFHpA		15.62	362.7 → 318.7	[^{13}C2]PFHxA
	Perfluorooctanoate	PFOA		17.59	412.7 → 368.7	[^{13}C4]PFOA
	Perfluorononanoate	PFNA		21.23	462.7 → 418.7	[^{13}C4]PFOA
	Perfluorodecanoate	PFDA		25.77	512.7 → 468.7	[^{13}C4]PFOA
	Perfluoroundecanoate	PFUnDA		32.57	562.7 → 518.7	[^{13}C2]PFDoDA
	Perfluorododecanoate	PFDoDA		36.49	612.7 → 568.7	[^{13}C2]PFDoDA
	Perfluorotridecanoate	PFTrDA		37.20	662.7 → 618.7	[^{13}C2]PFDoDA
	Perfluorotetradecanoate	PFTeDA		37.40	712.7 → 668.7	[^{13}C2]PFDoDA
PFSAs (perfluoroalkyl sulfonic acids)	Perfluorobutane sulfonate	PFBS	Tokyo Chemical Ind., 98%	13.34	298.7 → 98.7	[^{13}C4]PFOS
	Perfluorohexane sulfonate	PFHxS	Wellington Laboratories, 98%	21.40	398.7 → 98.7	[^{13}C4]PFOS
	Perfluorooctane sulfonate	PFOS	Kanto Chemical, 98%	15.58	498.7 → 98.7	[^{13}C4]PFOS
	Perfluorodecane sulfonate	PFDS	Wellington Laboratories, 98%	32.30	598.7 → 98.7	[^{13}C4]PFOS
Internal Standard (IS)	Perfluoro-n-[1,2,3,4-^{13}C2]butanoate	[^{13}C4]PFBA	Wellington Laboratories, 98%	6.26	216.7 → 171.7	–
	Perfluoro-n-[1,2-^{13}C2] hexanoate	[^{13}C2]PFHxA	Wellington Laboratories, 98%	14.12	314.7 → 269.6	–
	Perfluoro-n-[1,2,3,4-^{13}C4]octanoate	[^{13}C4]PFOA	Wellington Laboratories, 98%	17.66	416.7 → 371.6	–
	Perfluoro-n-[1,2-^{13}C2]dodecanoate	[^{13}C2]PFDoDA	Wellington Laboratories, 98%	36.53	614.6 → 569.6	–
	Perfluoro-1-[1,2,3,4-^{13}C4]octanesulfonate	[^{13}C4]PFOS	Wellington Laboratories, 98%	21.30	502.7 → 98.7	–

Supplementary Table 2. Instrumental parameters used for analytical determination of PFAAs

LC CONDITIONS								
Instrument	HP1100 (Agilent)							
Analytical column	Zorbax XDB C-18 (150 mm × 2.1 mm, aperture size 5 μm) (Agilent Tech., Santa Clara, USA)							
Mobile phase A	10mM Ammonium acetate aq.							
Mobile phase B	Methanol							
Flow rate	0.2 mL/min							
Gradient	Time (min)	0	5	15	25	31	42	44.5
	B (%)	10	62	65	70	100	70	10
Column Temp.	40 °C							
Injection Volume	10 μL							
TRIPLE QUADRUPOLE MS/MS CONDITIONS								
Instrument	Micromass Quattro Ultima (Waters, Milford, USA)							
Ionization	Electrospray ionization (ESI) in negative mode							
Gas temperature	350 °C							
Gas flow (N_2)	Cone: 50 L hr^{-1} ; Dissolvation: 500 L hr^{-1}							
Capillary voltage	2.70 kV							
Scan type	MRM							

Supplementary Table 3. Recoveries*, LODs and LOQs for individual PFAAs in surface water and sediment

PFAAs	% Recoveries [mean (RSD)]		LOD[a]		LOQ[b]		Linearity (r^2)[c]
	Water 10 ng/L (n=3)	Sediment 10 ng/g (n=3)	Water (ng/L)	Sediment (ng/g)	Water (ng/L)	Sediment (ng/g)	
PFBA	113 (6)	87 (1)	0.008	0.031	0.02	0.102	0.999
PFPeA	114 (3)	97 (5)	0.012	0.003	0.032	0.011	0.997
PFHxA	99 (5)	90 (4)	0.008	0.004	0.016	0.013	0.998
PFHpA	102 (6)	99 (4)	0.008	0.004	0.036	0.013	0.998
PFOA	94 (6)	102 (2)	0.120	0.023	0.40	0.076	0.999
PFNA	85 (5)	93 (6)	0.016	0.004	0.04	0.012	0.998
PFDA	83 (4)	95 (2)	0.008	0.002	0.036	0.006	0.999
PFUnDA	111 (6)	106 (3)	0.036	0.009	0.08	0.029	0.999
PFDoDA	93 (6)	107 (5)	0.040	0.003	0.08	0.011	0.999
PFTrDA	102 (2)	98 (5)	0.024	0.003	0.04	0.008	0.998
PFTeDA	95 (9)	103 (3)	0.024	0.002	0.04	0.007	0.999
PFBS	112 (3)	108 (5)	0.080	0.018	0.28	0.06	0.999
PFHxS	87 (4)	94 (5)	0.040	0.012	0.20	0.021	0.999
PFOS	104 (4)	98 (2)	0.080	0.026	0.10	0.088	0.999
PFDS	74 (2)	101 (5)	0.030	0.016	0.10	0.024	0.999

[a] Limit of detection;

[b] Limit of quantification;

[c] Calibration curves (0.01 – 50 µg/L for each compound);

*The spike recovery of PFASs was calculated using the equation: spike recovery = ($C_{sample + spiked}$ - C_{sample}) / C_{spiked} × 100%, where $C_{sample + spiked}$ is the concentration of PFASs in a spiked sample, C_{sample} is the concentration of PFASs in the sample (same as above without spiking target compounds), C_{spiked} is the concentration of the spiked target compound.

Supplementary Table 4. Comparison of PFAAs occurrence (ng/L) in studied rivers water with other rivers & lakes of the world. (value: minimum–maxmum (mean) or (mean ± standard deviation)

Rivers				
Location	**PFOA**	**PFOS**	**PFASs**	**References**
Buriganga River, Bangladesh	27.9–52.63 (39.34)	0.95–5.86 (2.88)	56.77–89.35 (71.12)	Present study
Shitalakkha River, Bangladesh	13.63–25.24 (18.74)	1.21–5.95 (3.58)	29.66–44.62 (37.32)	Present study
Turag River, Bangladesh	8.13–25.09 (17.23)	1.51–2.81 (1.98)	23.96–53.54 (42.22)	Present study
Seine River (NW France)			1.8–105	[1]
Chaobai River, Beijing	0.05–12.8	ND–4.40	0.04-31.3	[2]
Liuxi River, South China	10.9–74.0 (27.6)		506–3.16 × 10^3 (1.59 × 10^3)	[3]
Jiulong River and Xiamen Bay regions, China	(2.5)	(5.65)	10.48–149.29	[4]
Oder River, Europe		0.40–1.17	7.62–68.01	[5]
Swan Canning Estuary in Perth, Western Australia,		4.1–120 (27.3 ± 2.3)	(65.8 ± 5.9)	[6]
Truckee River, USA			(441.7)	[7]
LasVegasWash, USA			(2234.3)	[7]
Yangtze River Estuary, China				[8]
Rhône River, France	1.87–3.10			[9]
Fen River, China	2.49–4.79			[10]
Jucar River, Spain	0.07–52.2 (4.36)	0.01–128 (11.29)	21.1–1140 (91.8)	[11]
Ganges River, India	(0.39)	(0.54)	(10.86)	[12]
Xiaoqing River (Shandong)	1919.23–4534.41	0.73–3.28	2140.68–5068.97 (3455.78)	[13]
Yellow River (Shandong)	0.96–4.15	0.95–5.37	7.75–21.63 (13.21)	[13]
Llobregat River, Spain 2002-2005	<4.2–130	1.1–11.120		[14]
Llobregat River, Spain 2008-2012	4.9–44 (15)	20–348 (104)		[14]

València, Spain	0.99–120.2 (49.5)	0.94–58.1 (14.2)	0.99–120 (77.7)	[15]
Svitava Rivers, Czech Republic	8.1–9.1	9.5–12	(28.2)	[16]
Svratka Rivers, Czech Republic	1.7–3.1	0.6–0.65	(4.4)	[16]
Orge River, France	(9.4 ± 0.6)	(17.4 ± 2.2)	(73 ± 4.6)	[17]
Superior Lake, USA	0.24–1.2 (0.65)	0.1–0.4 (0.25)	1.14–5.25 (3.21)	[18]
Huron Lake, USA	0.66–4.72 (3.22)	0.24–5.46 (2.25)	3.26–19.17 (12.51)	[18]
Danube River, EU	(20)	(8)	(31)	[19]
Upper Mississippi River, USA	1.14–23.8 (5.85)	1.3–245(43.92)	4.79–369.36 (51.55)	[20]
Yamuna River, India	(0.09)	(1.81)		[21]
River Elbe, Germany	2.6–9.7	0.2–3.2		[22]
Chao Phraya River, Thailand	(4.7)	(1.9)		[23]
Bangpakong River, Thailand	(0.7)	(0.7)		[23]
Lake Victoria, Kenya	<0.4–96.4	<0.4–13.23		[24]
River Po, Italy	2–337	2–12	5–348	[25]
Kamo River, Japan	(36)	(4.1)		[26]
Uji River, Japan	100–110	8.7–10		[26]
Pearl River (Guangzhou)	0.85–13	0.9–99	31±37	[27]
Yangtze River (Shanghai)	2.0–260	<0.01–14	120±147	[27]
Xiaoqing River (Beijing)	(7.85)	(1.75)		[28]
Tennessee River, USA	<25–598	16.8–144		[29]
		Lakes		
Locations	**PFOA**	**PFOS**	**PFAAs**	**References**
Taihu Lake	2.15–73.85 (28.19)	<0.5–10.48 (3.53)	10.03–119.81 (56.86)	[30]
Nansi Lake	34.9–84.6	0.49–1.79	38.4–91.4 (67.05)	[31]
Lake Chaohu	(7.55±4.07)	(0.21±0.45)	(16.09±9.78)	[32]
Tangxun Lake	70.5–1390 (372)	73.4–1650 (357)	4570–11890 (9850)	[33]
Dianchi Lake	3.4–35.44	1.71–40.90	35.76–135.88	[34]

Supplementary Table 5. Comparison of PFAAs occurrence (ng/g dw) in studied rivers sediment with other rivers & lakes of the world. value: minimum–maximum (mean) or (mean ± standard deviation)

		Rivers		
Location	**PFOA**	**PFOS**	**PFASs**	**References**
Buriganga River, Bangladesh	0.06–0.18 (0.11)	0.72–8.25 (4.01)	3.24–11.67 (7.29)	Present study
Shitalakkha River, Bangladesh	0.09–0.15 (0.13)	0.33–2.01 (1.14)	2.86–5.40 (4.14)	Present study
Turag River, Bangladesh	<LOQ–0.17 (0.13)	0.21–4.13 (2.47)	2.18–6.98 (5.38)	Present study
Chaobai River, Beijing	ND–2.44	ND–3.26	0.03–4.29	[2]
Liuxi River, South China	ND–34.8 (5.28)		9.13–850	[3]
Jiulong River and Xiamen Bay regions, China			(3.21–7.41) 7.037	[4]
Jucar River, Spain	0.15–6.69 (1.32)	0.06–9.83 (1.71)	14.3–75.9 (21.8)	[11]
River Elbe, Germany	0.007–0.43 (0.093)	0.023–5.4 (0.5)	0.056–7.5 (1.0)	[35]
València, Spain	0.03–10.9 (3.19)	0.1–4.8 (1.79)	0.25–17.4 (6.22)	[15]
Orge River, France	(0.07)	(4.3 ± 0.3)	(8.4 ± 0.5)	[17]
Conasauga River, USA	0.06–1.97 (0.73)	1.73–20.18 (9.72)	0.29–39.2 (16.22)	[36]
Huangpu River, Shanghai, China	0.20–0.64 (0.43)	ND–0.42 (0.11)	0.25–1.10 (0.71)	[37]
Pearl River, Guangzhou, China	0.09–0.29 (0.21)	ND–3.1 (0.58)	0.09–3.60 (0.87)	[37]
Savannah River, USA	ND–0.2	0.3–0.8	0.5–3.6	[38]
Kamo River, Japan	(1.6)	(<1.9)	(2.54)	[26]
Uji River, Japan	1.3–3.9	(<1.4)	(4.75)	[26]
		Lakes		
Locations	**PFOA**	**PFOS**	**PFAAs**	**References**
Lake Chaohu, China	(0.10±0.03)	(0.09±0.05)	(10.64±0.23)	[39]
Taihu Lake, China	ND–0.85 (0.13)	0.13–6.95 (0.92)	1.11–8.21 (2.42)	[30]
Nansi Lake, China	0.11–0.44	0.17–0.83	0.47–1.81 (1.09)	[31]
Tangxun Lake, China	0.48–6.35 (2.35)	10.9–623 (74.4)	41.8–800 (151)	[33]
Dianchi Lake, China	ND–0.71	0.07–0.83	0.21–2.45	[34]
Superior Lake, USA	0.0–0.3 (0.1)	0.1–0.2 (0.1)	0.0–10.5 (1.5)	[40]
Huron Lake, USA	0.1–3.0 (0.5)	0.1–2.5 (0.9)	0.0–26.0 (3.1)	[40]

Supplementary Table 6. Risk quotients (PNEC) values of PFASs collected from the literature[41,42]

PFASs	Water (ng/L)	Sediment (ng/g)
PFBA	110000	241.316
PFPeA	32000	227.176
PFHxA	97000	2825.31
PFHpA	7852	1002.563
PFOA	1428	86
PFNA	1000000	255618.796
PFDA	45	51.488
PFUnDA	8	41.073
PFDoDA	1	32.024
PFTrDA	103	10644.855
PFTeDA	83	38325.704
PFBS	372000	1723.473
PFHxS	250000	388703.55
PFOS	610	4.9
PFDS	15400	1203.247

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