Supporting Information

A National-scale Study of Polycyclic Aromatic Hydrocarbons in Surface Water: Levels, Sources, and Carcinogenic Risk

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Table S1 Data sources of seven major Basins

No	Basins	Region	Water body	Sampling Points	Sampling time	PAH compounds	Reference
1	SRB	Heilongjiang	Surface water	14	Jun.2010	16	Wang, 2012
2		Jilin	River	9	2009–2010	16	Xu, 2011
3		Heilongjiang	River	15	2014	16	Zhao and Zhou, 2015
4		Heilongjiang	Reservoir	16	Jul.2010	15	Xiao et al., 2015
5		Jilin	River	25	2012	16	Liu, 2013
6		Heilongjiang	River	48	Jul.2010	16	Hu et al., 2017
7		Heilongjiang	River	21	May.2009	16	Ma et al., 2013
8		Jilin,Heilongjiang	River	42	Apr.Aug.2007	16	Zhao et al., 2014
9		Heilongjiang,Jilin	River	14	May.2009	16	Chen et al., 2016
10		Heilongjiang	River	10	Jan.May.2007	8	Sun et al., 2010
11		Inner Mongolia	River	18	Sep.2021	16	Qin et al., 2023
12		Inner Mongolia	River	45	Sep.2021	16	Qin et al., 2023
13		Heilongjiang	River	18	2010	15	Ma et al., 2012
14		Jilin	River	9	May.Aug.2013 Jan.2014	16	Zhang et al., 2015
15		Heilongjaing	River	14	Apr.Aug.2007 Jan.2008	16	Ding, 2008
16		Jilin	River	17	Nov.2014 May.Aug.2015	16	Sun et al., 2017

17	LRB	Liaoning	River	9	Jun.Sep.Nov.2009	16	Zheng et al,2010
18		Liaoning	Shallow groundwater	51	Dec.2014 Jul.2015	16	Xiang, 2020
19		Jilin	River	10	2012–2014	16	Su, 2014
20		Liaoning, Inner Mongolia	River	33	May.Oct.2012	16	Zhang et al., 2022
21		Liaoning, Inner Mongolia	River	20	Aug.2010	16	Zhang et al., 2012
22		Liaoning	River	27	Aug.2013	16	Wang et al., 2015
23		Liaoning	River	14	Apr.Jul.Nov.2009	16	Zhang et al., 2013
24		Liaoning	River	16	Aug.2005	16	Guo et al., 2007
25		Liaoning	River	50	2013	16	Bai et al., 2014
26		Liaoning	River	14	May.Aug.2015	16	H. Wang, et al., 2016
27		Liaoning	River	14	2011	16	Zhang et al., 2011
28		Liaoning	River	12	Aug.Nov.2007	16	Han et al., 2009
29		Liaoning	River	—	Aug.2005	16	Guo et al., 2011
30		Liaoning	River	10	Jul.Oct.2013 Jan.2014	16	Xie et al., 2015
31	HaRB	Beijing	Lake	5	Sep.2005 Mar.2006	16	Tong et al., 2007
32		Hebei	Lake	12	May.Aug.2015	17	Wang et al., 2017
33		Hebei,Beijing	River	47	Jun.2018	16	Zhou, 2019

34		Hebei	River	11	Jun.2019	16	Xing et al., 2019
35		Hebei	River	7	Apr.Aug.2008	16	Cao et al., 2010
36		Hebei	River	14	May.Aug.2015	16	Wang et al., 2017
37		Hebei	Lake	6	Oct.2007	15	Zhu et al., 2009
38		Beijing	River	62	Jul.2015 Mar.2016	16	Zhang et al., 2021
39		Hebei,Beijing	Reservoir	8	May.2012	16	Wang et al., 2015
40		Tianjin	River	30	2004	16	Shi et al., 2005
41		Shandong	River	5	Apr.2014	16	Wang et al., 2017
42		Hebei,Beijing,Tianjin	Reservoir	9	Apr.Aug.2017	16	Zhang et al., 2020
43	YRB	Henan	River	18	Jan.2007	15	Feng et al., 2015
44		Shaanxi	River and canal	38	Jul.2012	16	Wang et al., 2015
45		Henan	River	30	Jul.2018	16	Du et al., 2020
46		Shanxi	River	29	Aug.–Oct.2013	16	Zhao et al., 2017
47		Ningxia Hui Autonomous Region	River and Lake	15	Nov.2016 Mar.2017	16	Tian et al., 2019
48		Gansu	River	11	Nov.2004	16	Wang et al., 2007
49		Shandong	River	8	May.Sep.2005	16	Lang et al., 2008
50		Inner Mongolia	River	8	2012–2014	16	Zhang et al., 2016
51		Henan	River	12	Jun.Sep.2004	15	Li et al., 2006

52		Shaanxi	River	59	Oct.2021	16	Dong et al., 2022
53		Henan	River	26	Nov.2005 Aug.2006	16	Sun et al., 2009
54		Shandong	River	42	May.Aug.2007	16	Wang et al., 2009
55		Shaanxi	River	37	Aug.2014	16	Chen et al., 2015
56		Ningxia Hui Autonomous Region	River	13	Mar.2020	16	Jiang et al., 2023
57		Shaanxi	River	30	Oct.2020 May.2022	16	Zhou et al., 2023
58	HuRB	Shandong	Lake	9	Jul.2009	16	Zheng et al., 2010
59		Henan,Anhui	River	17	Dec.2013 Apr.Aug.2014	16	Liu, 2016
60		Anhui,Jiangsu	River	10	2009	15	Li et al., 2010
61		Henan,Anhui,Hebei	River	16	Dec.2013 Apr.Aug.2014	16	Liu et al., 2016
62		Anhui	River	12	Jul.2021	10	Zhang et al., 2023
63		Anhui	River	11	Aug.2011	16	Li, 2012
64		Anhui	River	5	Oct.2007	16	Zhao et al., 2009
65		Anhui	River	10	2021	16	Jiang et al., 2022
66	YtRB	Jiangsu	Lake	16	Jan.–Jul.2015	16	Li et al., 2018
67		Chongqing	River	8	Aug.2009	16	Cai et al., 2012
68		Anhui	Lake	15	Aug.2009	16	Qin et al., 2013

69	Chongqing	River	7	Oct.2010	15	Wang et al., 2015
70	Guizhou	Lake	15	Dec.2012	16	Liu et al., 2015
71	Hubei	River	8	Dec.2015	16	H. J. Wang, et al., 2016
72	Chongqing	River	28	Jun.–Dec.2014	16	Z. B. Wang, et al., 2016
73	Jiangsu	River	12	Jun.2019	16	Jia et al., 2020
74	Hubei	Lake	8	Aug.2015	16	Zhang et al., 2017
75	Yunnan, Sichuan, Hubei, Jaingxi, Jiangsu	River	19	Aug.2015	16	C. L. Wang, et al., 2016
76	Shanghai	Lake	17	Dec.2012	16	Guo et al., 2014
77	Guizhou	Lake	4	Sep.2009	16	Yu et al., 2010
78	Hubei	Underground river	9	Dec.2011, Jul.2012	16	Gong et al., 2015
79	Guizhou	Lake	8	2004	16	Luo, 2005
80	Zhejiang	River	13	2014	16	Bai et al., 2015
81	Hubei	River	30	Jul.Dec.2005	16	Feng et al., 2007
82	Anhui	River and Lake	28	Apr.2014	16	Li et al., 2016
83	Anhui	River	12	Dec.2015	16	Wu, 2017
84	Sichuan	River	20	Oct.2019	16	Chen et al., 2022
85	Chongqing	River	5	Aug.2010	16	Xu et al., 2012
86	Anhui	River	1	Jan.–Nov.2018-2020	15	Lin, 2023

87	PRB	Guangdong province	Aquatic water	12	May.–Dec.2013	16	Xie et al., 2014
88		Guangxi	Undergound River	8	Nov.2007	16	Kong et al., 2011
89		Guangdong	River	18	Jan.2013	16	Li et al., 2014
90		Guangxi	River	8	Aug.2017	16	Wang et al., 2019
91		Guangdong	River	13	Jul.2016	16	Han et al., 2018
92		Guangdong	River	4	Mar.2009	16	Wu et al., 2010
93		Guangdong	River	3	Jul.2004	16	Deng et al., 2006
94		Guangdong	Undergound River	5	2013–2014	16	Lu et al., 2018
95		Guangdong	River	24	Apr.2014	16	Xie et al., 2020

Table S2 Concentrations of 16 PAHs in seven major basins. (ng/L)

	Nap	Acy	Ace	Flu	Phe	Ant	Fla	Pyr	BaA	Chr	BbF	BkF	BaP	DahA	IcdP	BghiP
SRB	524.15	1512	1328.61	557.7	1509.76	304.14	607.58	437.95	70.2	121.29	140.1	71.94	353.22	8.1	3.37	2.09
LRB	208.54	15.95	17.06	57.18	187.44	101.43	127.74	122.67	193.3	77.46	70.26	28.75	60.78	70.74	21.12	30.81
HaRB	61.25	6.11	14.04	21.63	50.44	15.31	23.48	14.51	35.42	11.18	12.92	8.9	8.48	2.34	7.6	6.47
YRB	221.19	42.06	86.71	97.54	164.59	24.45	53.38	53.04	56.21	70.07	37.62	21.65	31.27	41.79	30.85	40.71
HuRB	621.36	470.11	23.81	68.87	226.42	36.23	35.08	41.96	82.11	47.31	28.46	6.61	16.57	7.45	22.24	9.11
YtRB	81.3	21.25	28.1	40.42	109.02	45.64	54.89	56.95	34.96	37.07	21.65	18.75	26.77	6.6	13.86	10.02
PRB	241.62	25.73	10.65	19.14	46.99	9.19	12.64	8.18	3.73	4.23	4.9	6.44	5.2	2.44	3.88	5.19
MAX	3463.8	11275.87	7555.13	3700	11300	2340	4660	3070	1266.46	650	1050	520	2789.9	683.82	152.3	304.44
MIN	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
SD	460.83	1241.35	858	402.73	1218.15	276.86	508.73	341.55	167.66	117.53	138.32	73.15	308.63	79.22	33.49	47.62

Note:"nd" indicates that it is not checked out.

SRB: Songhua River Basin; LRB: Liaohe River Basin; HaRB: Haihe River Basin; YRB: Yellow River Basin; HuRB: Huaihe River Basin; YtRB: Yangtze River Basin; PRB: Pearl River Basin

Table S3 Physical and chemical properties of PAHs.

PAHs	Abbr.	Ring	Molecular formula	Melting point (℃)	Boiling point (℃)	Water solubility(mg/L)	$logK_{ow}$
Naphthalene	Nap	2	$C_{10}H_8$	80.5	218	31.7	3.33
Acenaphthylene	Acy	3	$C_{12}H_8$	92-93	280	3.93	4.07
Acenaphthene	Ace	3	$C_{12}H_{10}$	96.2	279	1.93	3.98
Fluorene	Flu	3	$C_{13}H_{10}$	116	295	1.68-1.98	4.18
Phenanthrene	Phe	3	$C_{14}H_{10}$	101	340	1.2	4.45
Anthracene	Ant	3	$C_{16}H_{10}$	218	340	0.076	4.45
Fluoranthene	Fla	4	$C_{16}H_{10}$	111	383	0.2-0.26	4.9
Pyrene	Pyr	4	$C_{18}H_{12}$	156	404	0.0013	4.88
Benzo[a]anthracene	BaA	4	$C_{18}H_{12}$	158-159	448	0.01	5.61
Chrysene	Chr	4	$C_{18}H_{12}$	255-256	435	0.0028	5.16
Benzo[b]fluoranthene	BbF	5	$C_{20}H_{12}$	168.3	481	0.0012	6.04
Benzo[k]fluoranthene	BkF	5	$C_{20}H_{12}$	215.7	481	0.00076	6.04
Benzo[a]pyrene	BaP	5	$C_{20}H_{12}$	179-179.3	496	0.0023	6.06
Dibenzo[a,h]anthracene	DahA	5	$C_{22}H_{14}$	262	535	0.0025	6.84
Benzo[g,h,i]perylene	BghiP	6	$C_{22}H_{12}$	273	542	0.062	6.5
Indeno[1,2,3-cd]pyrene	IcdP	6	$C_{22}H_{12}$	163.6	534	$2.6x10^{-7}$	6.58

Table S4-1 Toxic equivalent concentration of seven carcinogenic monomers in seven major basins. (ng/L)

carcinogenic PAHs	BaA	Chr	BbF	BkF	BaP	DahA	IcdP	Mean	SD
SRB	7.02	1.21	14.01	7.19	353.22	8.01	0.34	390.99	986.52
LRB	19.33	0.77	7.03	2.87	60.78	70.74	2.11	163.63	396.95
HaRB	3.54	0.11	1.29	0.89	8.48	2.34	0.76	17.42	35.21
YRB	5.6	0.7	3.76	2.16	31.27	41.79	3.08	88.36	149.42
HuRB	8.21	0.47	2.85	0.66	16.57	7.45	2.22	38.44	52.94
YtRB	3.5	0.37	2.16	1.88	26.77	6.05	1.39	42.12	101.41
PRB	0.37	0.04	0.49	0.64	5.2	2.44	0.39	9.57	9.02

SD is the standard deviation.

Table S4-2 Monte Carlo model results for carcinogenic risk assessment in seven major basins (Children).

	SRB	LRB	HaRB	YRB	HuRB	YtRB	PRB
Mean	1.36×10^{-6}	6.78×10^{-7}	6.21×10^{-8}	3.22×10^{-7}	1.50×10^{-7}	1.42×10^{-7}	3.88×10^{-8}
Median	3.16×10^{-7}	1.27×10^{-7}	1.70×10^{-8}	9.36×10^{-8}	4.77×10^{-8}	3.73×10^{-8}	1.48×10^{-8}
Coeff. of Variation	3.05	4.45	3.18	2.51	2.42	2.32	2.93
Minimum	6.09×10^{-10}	6.61×10^{-10}	1.62×10^{-10}	4.47×10^{-10}	3.70×10^{-10}	2.15×10^{-10}	1.58×10^{-10}
Maximum	6.57×10^{-5}	7.68×10^{-5}	4.73×10^{-6}	1.48×10^{-5}	6.08×10^{-6}	5.18×10^{-6}	2.86×10^{-6}
Mean Std. Error	1.31×10^{-5}	9.55×10^{-8}	6.24×10^{-9}	2.56×10^{-8}	1.15×10^{-8}	1.04×10^{-8}	3.59×10^{-9}
Percentiles							
5%	1.5×10^{-8}	7.23×10^{-9}	1.14×10^{-9}	7.06×10^{-9}	3.90×10^{-9}	2.56×10^{-9}	1.48×10^{-9}
10%	2.88×10^{-8}	1.36×10^{-8}	1.97×10^{-9}	1.37×10^{-8}	7.11×10^{-9}	4.26×10^{-9}	2.62×10^{-9}
50%	3.15×10^{-7}	1.27×10^{-7}	1.70×10^{-8}	9.34×10^{-8}	4.76×10^{-8}	3.72×10^{-8}	1.48×10^{-8}
75%	9.6×10^{-7}	4.36×10^{-7}	5.09×10^{-8}	2.61×10^{-7}	1.36×10^{-7}	1.24×10^{-7}	3.74×10^{-8}
90%	2.92×10^{-6}	1.30×10^{-6}	1.39×10^{-7}	6.97×10^{-7}	3.40×10^{-7}	3.32×10^{-7}	8.74×10^{-8}
95%	5.17×10^{-6}	2.57×10^{-6}	2.41×10^{-7}	1.48×10^{-6}	5.60×10^{-7}	6.26×10^{-7}	1.26×10^{-7}

Table S4-3 Monte Carlo model results for carcinogenic risk assessment in seven major basins (Teenagers).

	SRB	LRB	HaRB	YRB	HuRB	YtRB	PRB
Mean	1.93×10^{-6}	6.18×10^{-7}	9.18×10^{-8}	4.41×10^{-7}	2.02×10^{-7}	1.85×10^{-7}	5.81×10^{-8}
Median	4.30×10^{-7}	1.76×10^{-7}	2.13×10^{-8}	1.35×10^{-7}	6.98×10^{-8}	4.72×10^{-8}	2.53×10^{-8}
Coeff. of Variation	2.76	2.47	5.46	2.42	2.38	3.29	1.86
Minimum	2.48×10^{-9}	9.63×10^{-10}	2.04×10^{-10}	1.45×10^{-9}	8.54×10^{-10}	2.13×10^{-10}	4.87×10^{-10}
Maximum	6.64×10^{-5}	2.31×10^{-5}	1.45×10^{-5}	1.50×10^{-5}	8.05×10^{-6}	1.10×10^{-5}	1.72×10^{-6}
Mean Std. Error	1.68×10^{-7}	4.83×10^{-8}	1.59×10^{-8}	3.38×10^{-8}	1.52×10^{-8}	1.92×10^{-8}	3.42×10^{-9}
Percentiles							
5%	2.9×10^{-8}	1.1×10^{-8}	1.63×10^{-9}	1.16×10^{-8}	7.49×10^{-9}	2.62×10^{-9}	3.26×10^{-9}
10%	4.53×10^{-8}	2.02×10^{-8}	2.96×10^{-9}	2.08×10^{-8}	1.06×10^{-8}	5.09×10^{-9}	5.00×10^{-9}
50%	4.3×10^{-7}	1.76×10^{-7}	2.12×10^{-8}	1.35×10^{-7}	6.97×10^{-8}	4.71×10^{-8}	2.52×10^{-8}
75%	1.37×10^{-6}	5.41×10^{-7}	6.26×10^{-8}	4.07×10^{-7}	1.91×10^{-7}	1.36×10^{-7}	6.10×10^{-8}
90%	4.59×10^{-6}	1.34×10^{-6}	1.70×10^{-7}	1.02×10^{-6}	4.73×10^{-7}	3.74×10^{-7}	1.33×10^{-7}
95%	9.12×10^{-6}	2.76×10^{-6}	2.95×10^{-7}	1.56×10^{-6}	7.61×10^{-7}	7.14×10^{-7}	2.09×10^{-7}

Table S4-4 Monte Carlo model results for carcinogenic risk assessment in seven major basins (Adults).

	SRB	LRB	HaRB	YRB	HuRB	YtRB	PRB
Mean	6.19×10^{-6}	2.12×10^{-6}	2.40×10^{-7}	1.20×10^{-6}	5.77×10^{-7}	6.76×10^{-7}	1.40×10^{-7}
Median	1.57×10^{-6}	6.25×10^{-7}	7.46×10^{-8}	4.68×10^{-7}	2.39×10^{-7}	1.63×10^{-7}	7.46×10^{-8}
Coeff. of Variation	2.94	2.93	2.48	2.16	1.86	3.69	1.47
Minimum	8.7×10^{-9}	3.17×10^{-9}	2.48×10^{-10}	7.58×10^{-9}	3.85×10^{-9}	1.98×10^{-9}	2.40×10^{-9}
Maximum	3.8×10^{-4}	1.37×10^{-4}	9.46×10^{-6}	3.16×10^{-5}	1.62×10^{-5}	5.01×10^{-5}	2.48×10^{-6}
Mean Std. Error	5.76×10^{-7}	1.96×10^{-7}	1.88×10^{-8}	8.19×10^{-8}	3.40×10^{-8}	7.88×10^{-8}	6.49×10^{-9}
Percentiles							
5%	1.13×10^{-7}	5.18×10^{-8}	6.91×10^{-9}	4.94×10^{-8}	2.47×10^{-8}	1.36×10^{-8}	1.20×10^{-8}
10%	2.05×10^{-7}	8.87×10^{-8}	1.20×10^{-8}	8.12×10^{-8}	4.37×10^{-8}	2.41×10^{-8}	1.73×10^{-8}
50%	1.56×10^{-6}	6.24×10^{-7}	7.45×10^{-8}	4.68×10^{-7}	2.39×10^{-7}	1.63×10^{-7}	7.54×10^{-8}
75%	5.20×10^{-6}	1.74×10^{-6}	2.06×10^{-7}	1.17×10^{-6}	6.45×10^{-7}	4.74×10^{-7}	1.63×10^{-7}
90%	1.42×10^{-5}	4.42×10^{-6}	5.73×10^{-7}	2.49×10^{-6}	1.39×10^{-6}	1.38×10^{-6}	3.13×10^{-7}
95%	2.46×10^{-5}	8.38×10^{-6}	1.04×10^{-6}	4.22×10^{-6}	2.11×10^{-6}	2.29×10^{-6}	4.64×10^{-7}

Table S4-5 Values and probability distributions of parameters.

Parameters	Units	Distribution	Children (0–10 years)	Teenagers (11–20 years)	Adults (21–70 years)
IR [a c]	$L \cdot d^{-1}$	Lognormal	1.28, 1.69	1.44, 1.69	1.85, 1.56
BW [b e]	Kg	Normal	23.03, 1.01	52.23, 1.04	59.25, 1.05
EF [c]	$d \cdot a^{-1}$	Triangle	180, 345, 365	180, 345, 365	180, 345, 365
ED [c f]	A	Triangle	0, 6, 10	11, 14, 20	21, 30, 70
AT [a]	D	——	25550	25550	25550
CSF [c]	$Kg \cdot D \cdot mg^{-1}$	——	1	1	1

[a] Adapted from USEPA;

[b] Adapted from Department of Health, ROC (http://www.doh.gov.tw/cht/index.aspx#);

[c] Adapted from USEPA 2017;

[d] Adapted from Ma et al., 2013;

[e] Adapted from Liao and Chiang, 2006;

[f] Adapted from Yang et al., 2014.

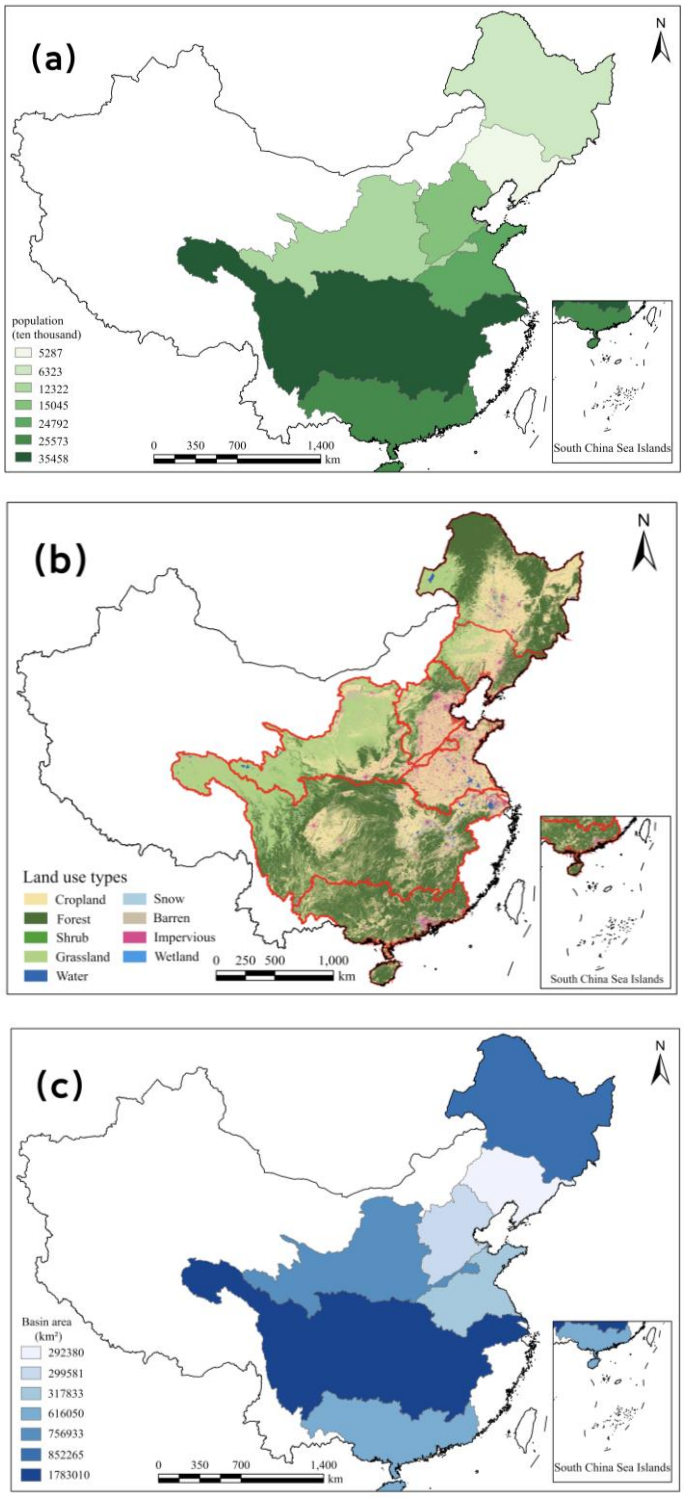


Figure. S1. Population (a), land use types (b), and basin area (c) of the seven main river basins in China.

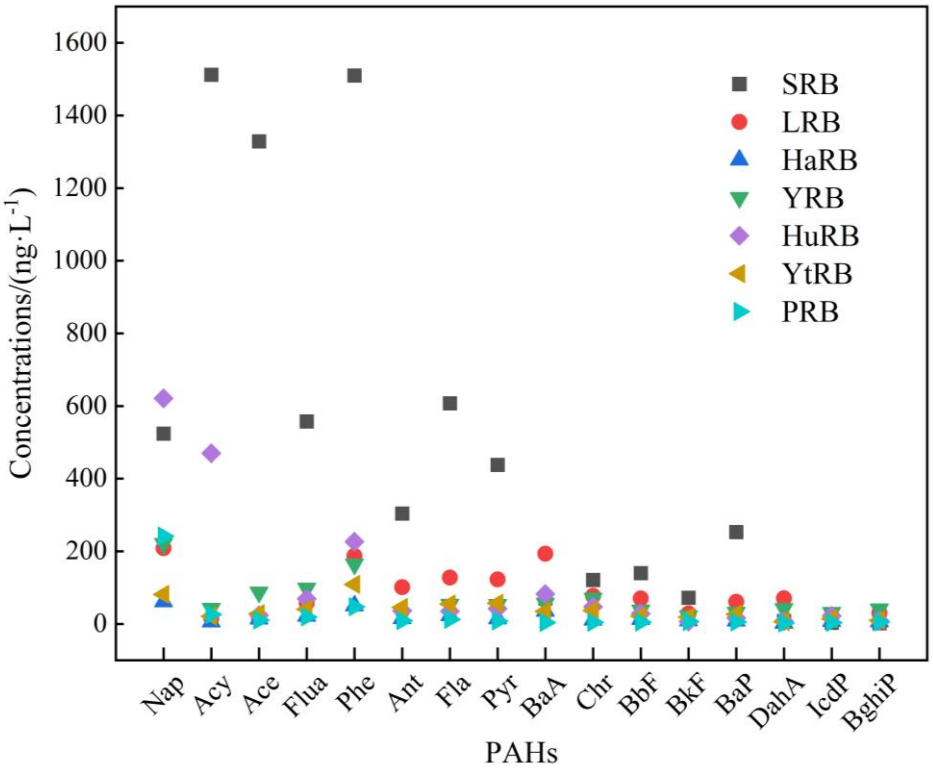


Figure. S2. Concentrations of 16 PAH compounds in the surface water of seven main river basins across China.

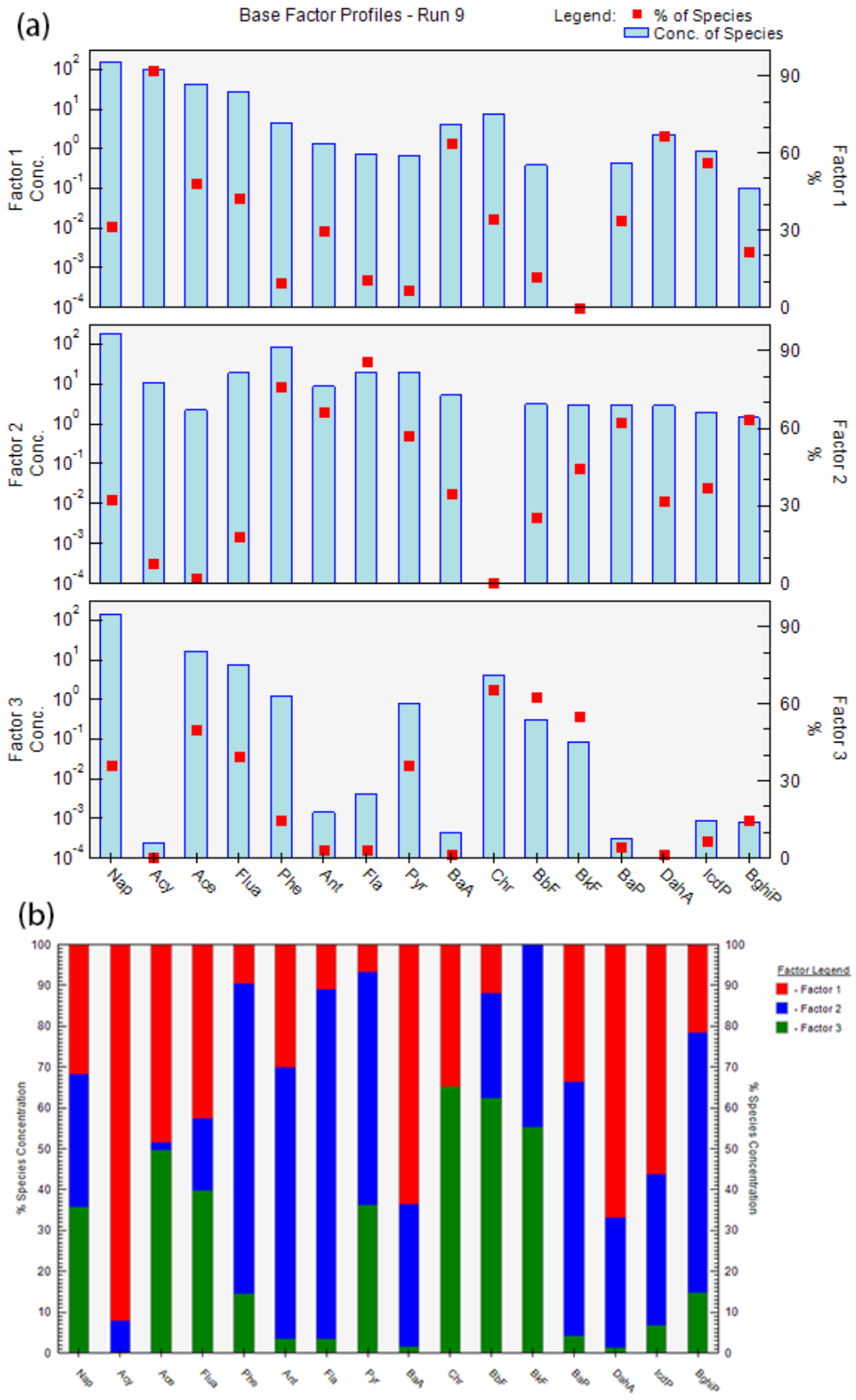


Figure. S3. Fractional source concentrations (a) and average source contributions of individual PAH species (b) from PMF model in water from SRB.

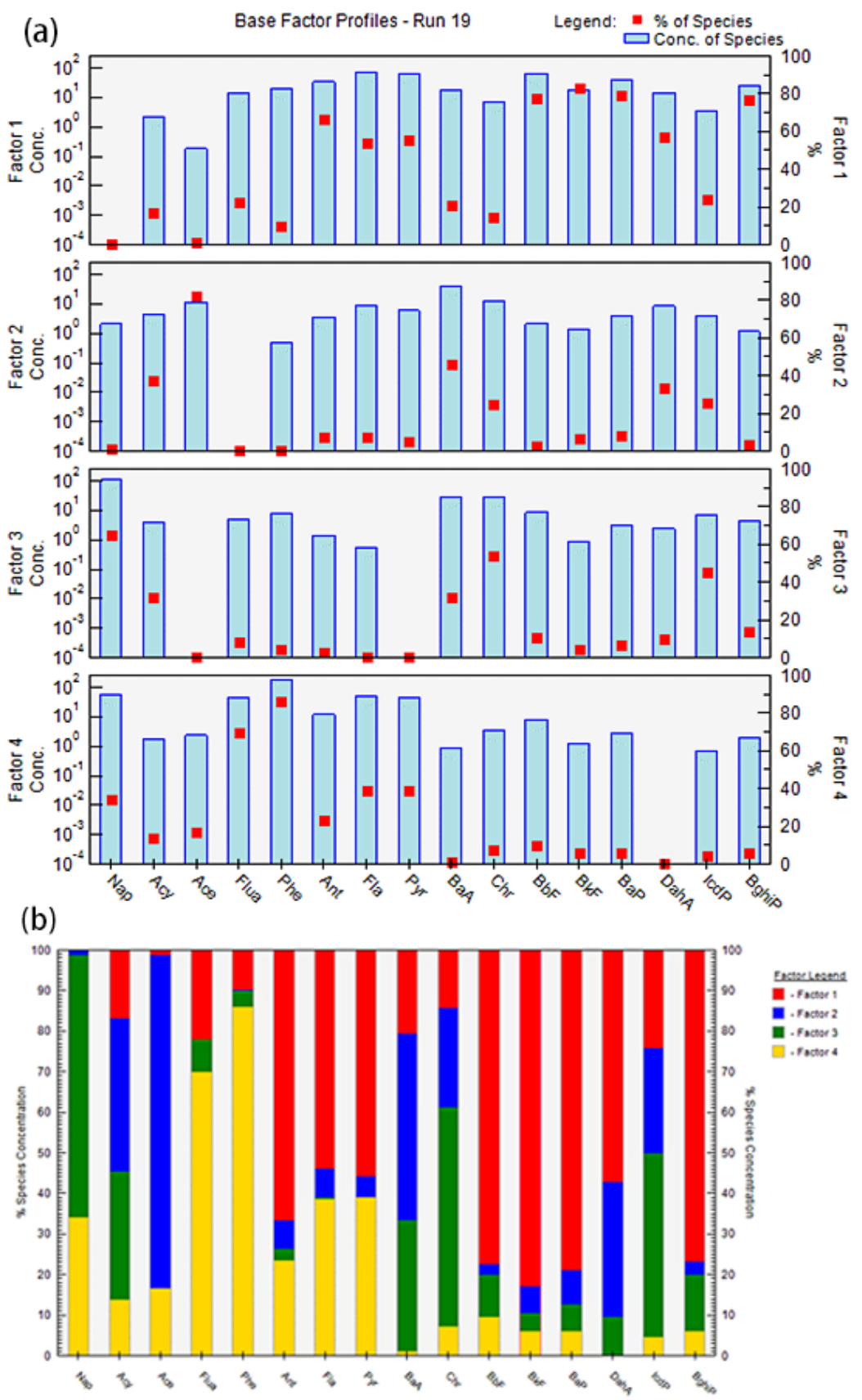


Figure. S4. Fractional source concentrations (a) and average source contributions of individual PAH species (b) from PMF model in water from LRB.

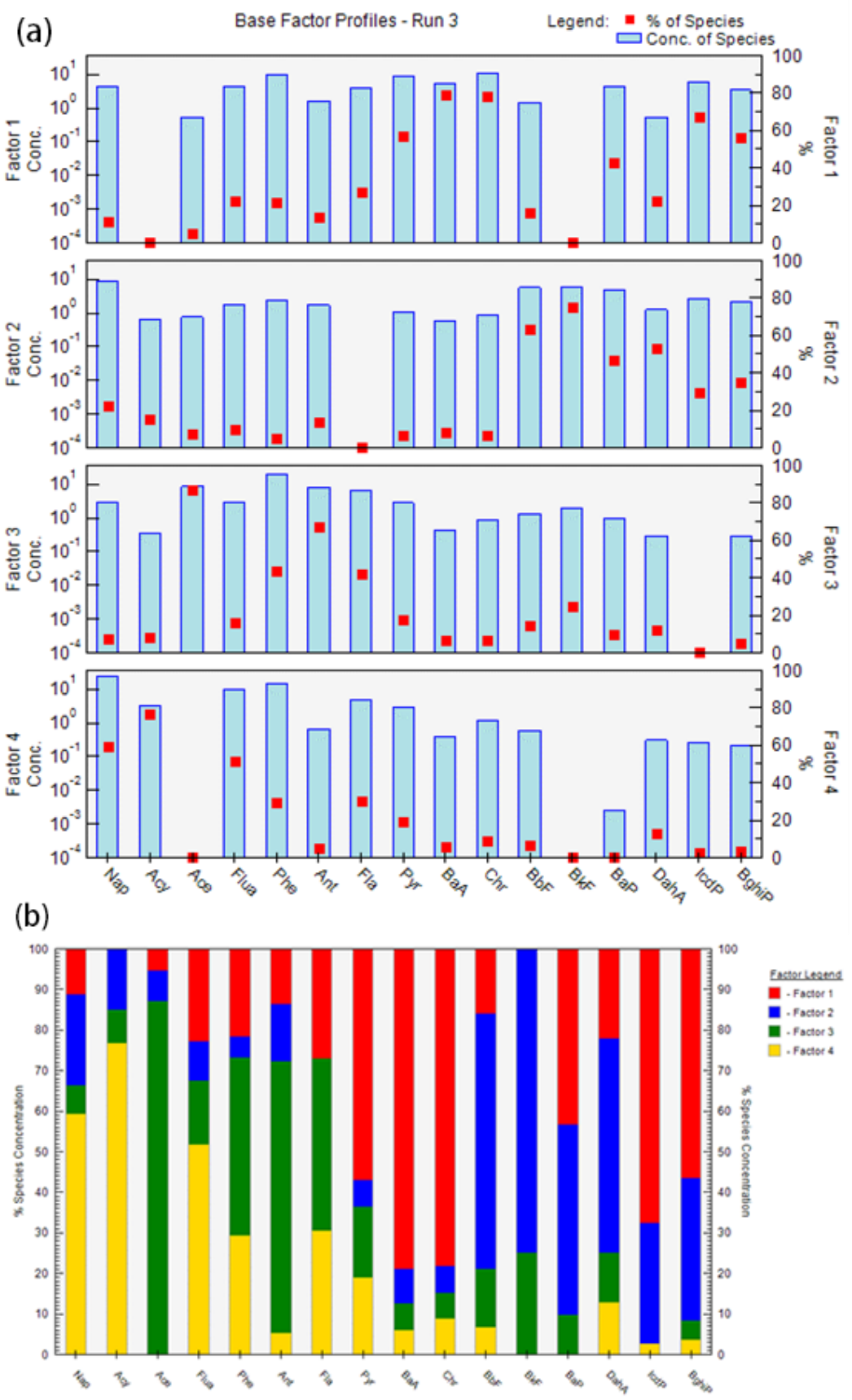


Figure. S5. Fractional source concentrations (a) and average source contributions of individual PAH species (b) from PMF model in water from HaRB.

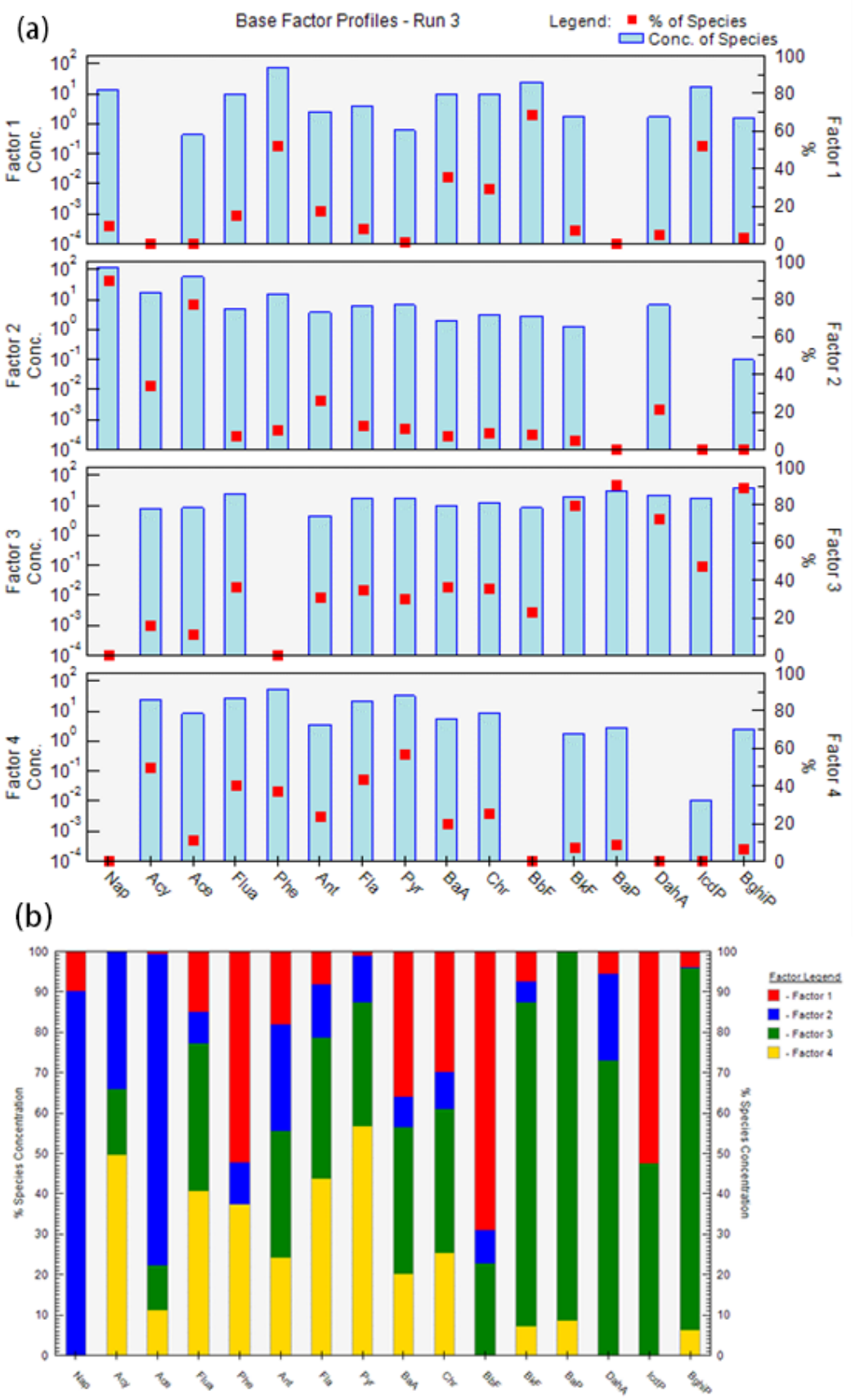


Figure. S6. Fractional source concentrations (a) and average source contributions of individual PAH species (b) from PMF model in water from YRB.

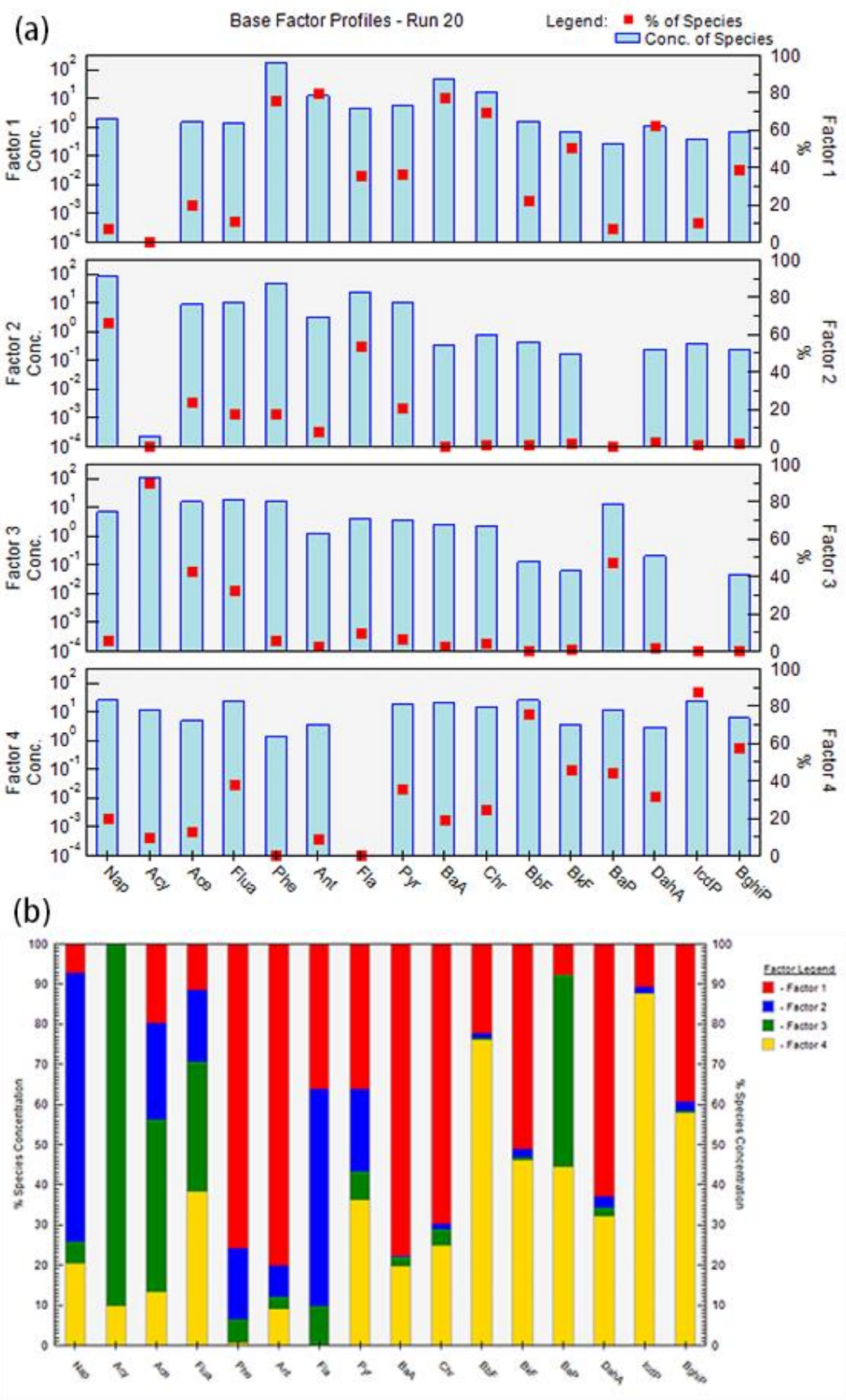


Figure. S7. Fractional source concentrations (a) and average source contributions of individual PAH species (b) from PMF model in water from HuRB.

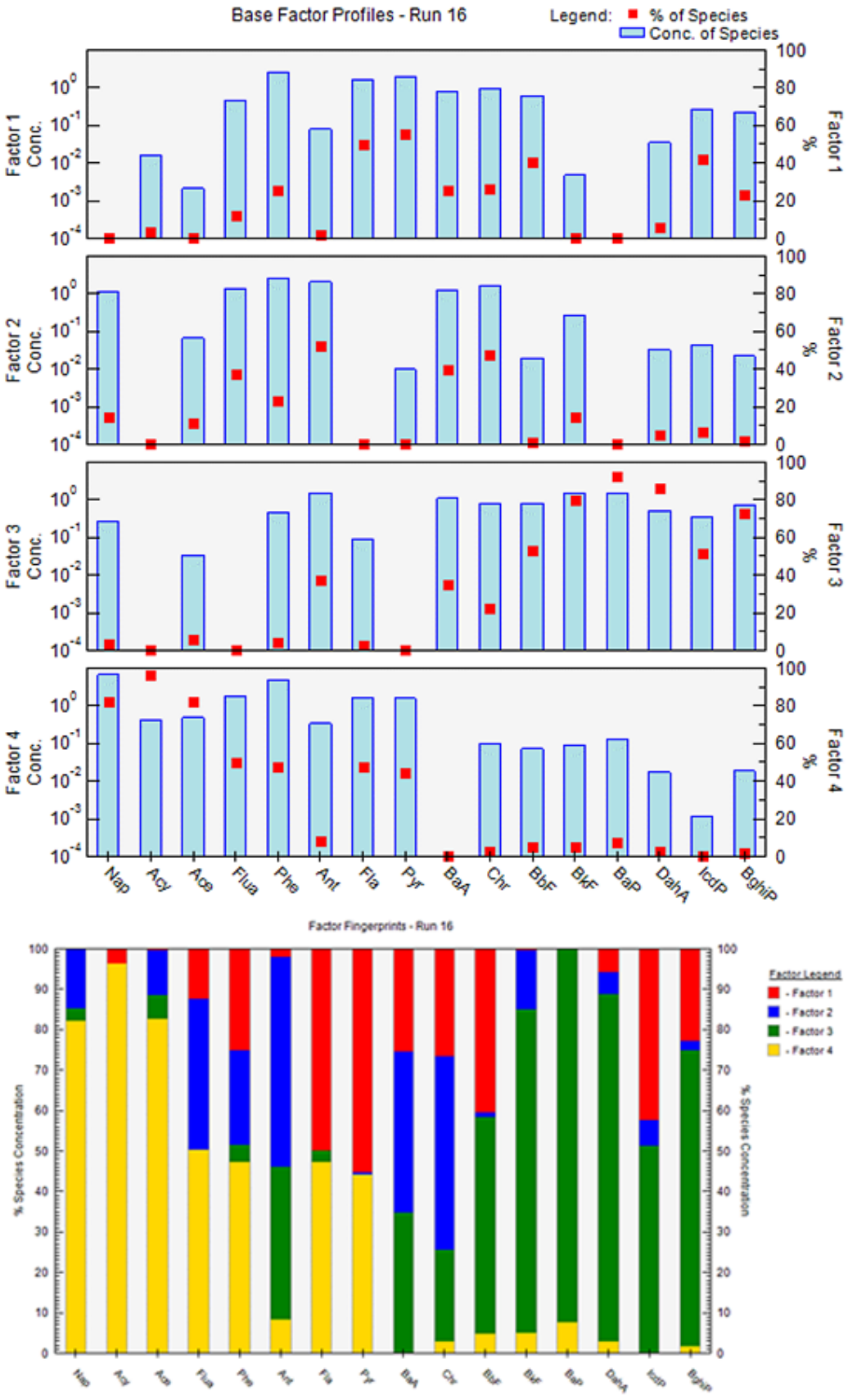


Figure. S8. Fractional source concentrations (a) and average source contributions of individual PAH species (b) from PMF model in water from YtRB.

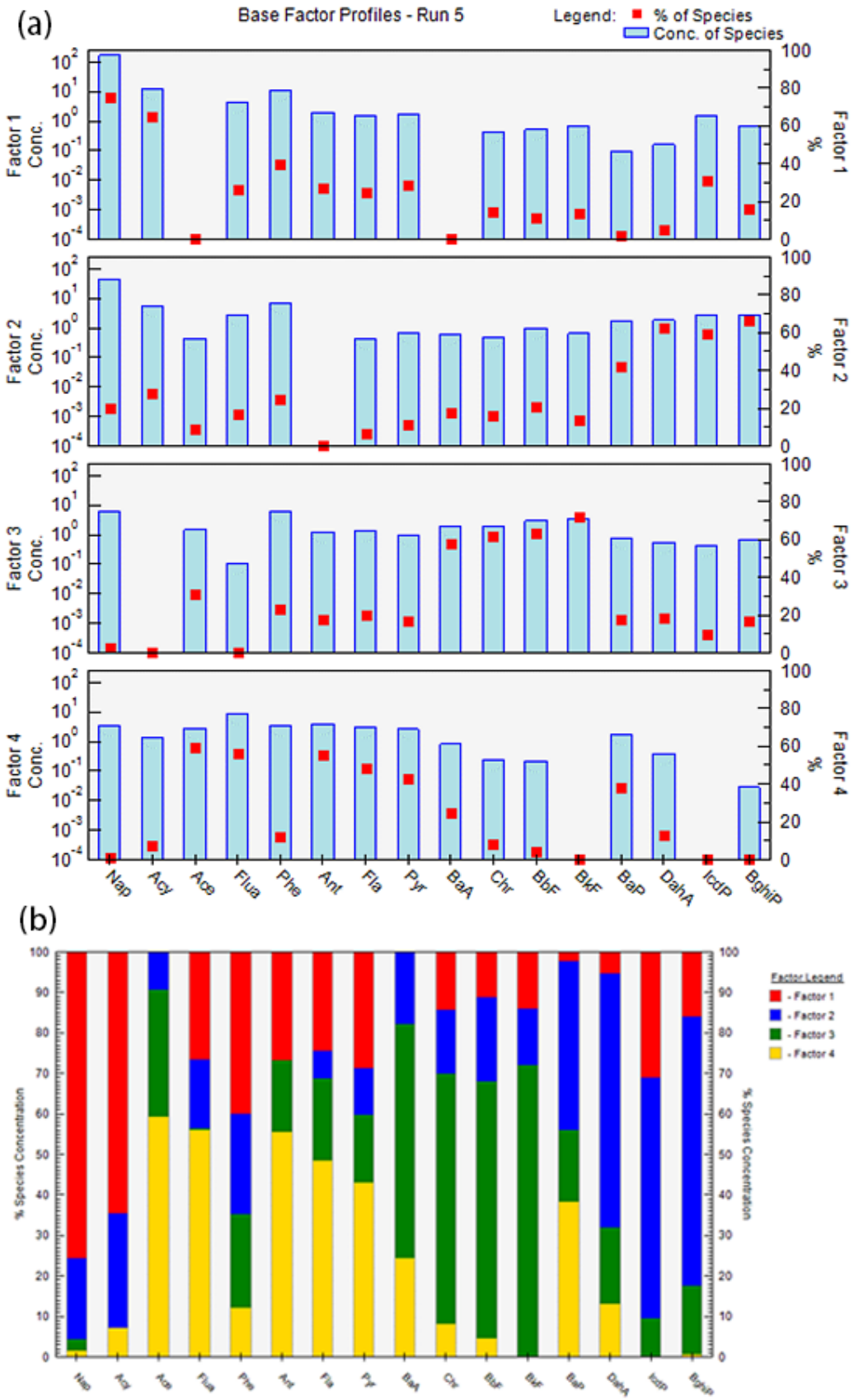


Figure. S9. Fractional source concentrations (a) and average source contributions of individual PAH species (b) from PMF model in water from PRB.

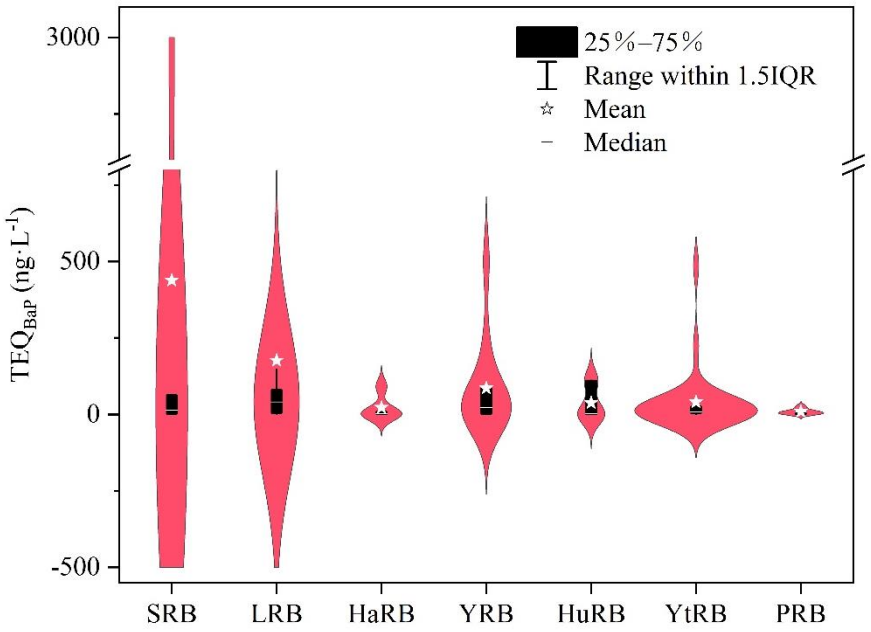


Figure. S10. Organ chart of TEQ_{BaP} in the surface water of seven main river basins across China.

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