

Supplementary Material

Table S1 The detail information of five sample sites

Sample sites	River	Longitude	Latitude	Sample types	Sampled date
A	Yongding River	115.618858°E	40.229813°N	surface sediment	October, 2016
B	Wenyu River	116.462835°E	40.145276°N	surface sediment	October, 2016
C	Ju River	117.041429°E	40.075949°N	surface sediment	October, 2016
D	Beiyun River	116.916628°E	39.77514°N	surface sediment	October, 2016
E	Dashi River	116.100728°E	39.588825°N	surface sediment	October, 2016

Table S2 The information of target compounds

Compounds	Abbreviation	CASN	Place of origin
PAHs(15 PAHs Mix, AccuStandard, > 99%,GC)			
Naphthalene	NAP	91-20-3	J&K Chemical company, USA
Acenaphthylene	ACEY	208-96-8	J&K Chemical company, USA
Acenaphthene	ACE	83-32-9	J&K Chemical company, USA
Fluorene	FLUO	86-73-7	J&K Chemical company, USA
Phenanthrene	PHE	85-01-8	J&K Chemical company, USA
Anthracene	AN	120-12-7	J&K Chemical company, USA
Fluoranthene	FLUOAN	206-44-0	J&K Chemical company, USA
Pyrene	PY	129-00-0	J&K Chemical company, USA
Benz[a]anthracene	BaAN	56-55-3	J&K Chemical company, USA
Benzo[b]fluoranthene	BbF	205-99-2	J&K Chemical company, USA
Benzo[k]fluoranthene	BkF	207-08-9	J&K Chemical company, USA
Benzo[a]pyrene	BaP	50-32-8	J&K Chemical company, USA
Indeno[1,2,3,cd]pyrene	INPY	95050-14-9	J&K Chemical company, USA
Dibenz[a,h]anthracene	DiBAN	53-70-3	J&K Chemical company, USA
Benzo[g,h,i]perylene	BPER	191-24-2	J&K Chemical company, USA
PAEs(15 PAEs Mix, AccuStandard, > 99%,GC)			
Dimethyl phthalate	DMP	131-11-3	J&K Chemical company, USA
Diethyl phthalate	DEP	84-66-2	J&K Chemical company, USA
Diisobutyl phthalate	DIBP	84-69-5	J&K Chemical company, USA
Di-n-butyl phthalate	DNBP	84-74-2	J&K Chemical company, USA
Bis(2-methoxyethyl)phthalate	DMEP	117-82-8	J&K Chemical company, USA
Bis(2-ethoxyethyl)phthalate	DEEP	605-54-9	J&K Chemical company, USA
Diamyl phthalate	DPP	131-18-0	J&K Chemical company, USA
Dihexyl phthalate	DHP	84-75-3	J&K Chemical company, USA
Bis(4-methyl-2-pentyl)phthalate	DMPP	146-50-9	J&K Chemical company, USA
Butyl benzyl phthalate	DBBP	85-68-7	J&K Chemical company, USA
Dicylohexyl phthalate	DCHP	84-61-7	J&K Chemical company, USA
Bis(2-n-butoxyethyl)phthalate	DBEP	117-83-9	J&K Chemical company, USA
Bis(2-ethylhexyl)phthalate	DEHP	117-81-7	J&K Chemical company, USA
Di-n-octyl phthalate	DNOP	117-84-0	J&K Chemical company, USA
Dinonyl phthalate	DNP	84-76-4	J&K Chemical company, USA
OCPs(19 OCPs Mix, AccuStandard, > 99%,GC)			
α -BHC		319-84-6	J&K Chemical company, USA

β-BHC		319-85-7	J&K Chemical company, USA
γ-BHC		55963-79-6	J&K Chemical company, USA
δ-BHC		319-86-8	J&K Chemical company, USA
Heptachlor		76-44-8	J&K Chemical company, USA
Aldrin		309-00-2	J&K Chemical company, USA
Heptachlor epoxide		1024-57-3	J&K Chemical company, USA
γ-chlordane		57-74-9	J&K Chemical company, USA
α-chlordane		5103-71-9	J&K Chemical company, USA
p,p'-DDE	DDE	72-55-9	J&K Chemical company, USA
Dieldrin		60-57-1	J&K Chemical company, USA
Endrin		72-20-8	J&K Chemical company, USA
p,p'-DDD		72-54-8	J&K Chemical company, USA
p,p'-DDT		50-29-3	J&K Chemical company, USA
Methoxychlor		72-43-5	J&K Chemical company, USA
Endosulfan I		959-98-8	J&K Chemical company, USA
Endosulfan sulfate		1031-07-8	J&K Chemical company, USA
Endrin aldehyde		7421-93-4	J&K Chemical company, USA
Endrin ketone		53494-70-5	J&K Chemical company, USA
Es(6 Es Mix, AccuStandard, > 99%,GC)and BPA (> 99.0%, GC)			
17-β-estradiol	E1	50-28-2	J&K Chemical company, USA
Estrone	E2	53-16-7	J&K Chemical company, USA
Estriol	E3	50-27-1	J&K Chemical company, USA
17-α-Ethinylestradiol	EE2	57-63-6	J&K Chemical company, USA
Diethylestradiol	DES	56-53-1	J&K Chemical company, USA
Estradiol valerate	EV	979-32-8	J&K Chemical company, USA
Bisphenol A	BPA	80-05-7	J&K Chemical company, USA

Table S3 Temperature programming parameters for different compounds

	Initial temperature(°C)	Rate (°C/min)	Final temperature(°C)	Holding time(min)
PAHs	40	-	-	2
	40	10	300	5
	60	-	-	2
OCPs	60	20	120	-
	120	10	180	-
	180	2	190	-
	190	15	300	3
PAEs	100	-	-	2
	100	20	180	2
	180	5	250	2
	250	10	280	10
Es and BPA	100	-	-	2
	100	25	180	5
	180	10	300	5

Table S4 The concentration of the blank control of the overall pretreatment and analysis process (ng·g⁻¹, dry weight)

Compounds	Concentration
PAHs(15)	
NAP	3.5
ACEY	0.0
ACE	0.7
FLUO	2.5
PHE	9.2
AN	1.5
FLUOAN	3.5
PY	3.1
BaAN	1.8
BbF	2.7
BkF	1.4
BaP	1.7
INPY	4.0
DiBAN	3.7
BPER	3.1
OCP(1)	
P,P'-DDE	0.9
PAEs(5)	
DMP	18.9
DEP	290.1
DIBP	178.1
DNBP	58.8
DNOP	37.0
Estrogen and BPA	
BPA	0.5
DES	0.9

Table S5 Quality control information

No.	Compounds	MQL(ng·g ⁻¹)	r ²	Recovery%	SD% (n = 6)
PAHs					
1	NAP	1	0.9996	69.28	1.53
2	ACEY	1	0.9974	60.32	7.39
3	ACE	1	0.9991	62.81	9.62
4	FLUO	1	0.9992	77.94	9.95
5	PHE	1	0.9995	110.77	5.33
6	AN	1	0.9962	74.63	6.14
7	FLUOAN	1	0.9983	106.09	0.36
8	PY	1	0.9983	96.66	1.84
9	BaA	1	0.9918	102.81	1.69
10	CHRY	1	0.998	104.93	2.62
11	BbF	5	0.994	114.06	1.09
12	BkF	5	0.997	102.03	0.12
13	BaPY	10	0.9925	88.9	2.83

14	INPY	10	0.9908	118.09	2.3
15	DiBAN	10	0.9918	118.38	0.72
16	BPER	10	0.9935	109.19	2.1
OCPs					
1	α -BHC	1	0.9994	86.02	4.79
2	β -BHC	2.5	0.9991	119.84	8.48
3	γ -BHC	2.5	0.9991	85.76	3.26
4	S-BHC	2.5	0.9952	114.73	1.32
5	Heptachlor	5	0.9992	66.34	7.93
7	Heptachlor epoxide	1	0.9974	94.99	5.03
8	Trans-chlordane	2.5	0.9978	91.82	3.99
9	Cis-chlordane	1	0.9992	88.81	4.47
10	P,P'-DDE	1	0.9984	90.71	2.29
11	Dieldrin	1	0.9996	102.82	0.62
12	Endrin	10	0.9982	66.92	2.41
13	Endosulfan	2.5	0.9958	99.99	2.43
14	P,P'-DDD	1	0.9917	90.29	2.68
15	Endrin aldehyde	2.5	0.9927	85.96	7.65
16	Endosulfate	10	0.9929	114.21	2.5
17	P,P'-DDT	1	0.994	90.34	5.5
18	Endrin ketone	5	0.9934	75.05	3.12
PAEs					
1	DMP	10	0.991	74.28	7.95
2	DEP	10	0.998	117.91	3.71
3	DIBP	10	0.991	118.11	1.96
4	DNBP	10	0.9929	107.24	2.07
5	DMEP	10	0.9929	64.66	5.84
6	DMPP	10	0.9933	80.52	11.57
7	DEEP	10	0.9915	74.46	4.48
8	DPP	10	0.9925	71.33	4.55
9	DHP	10	0.9905	80.25	9.2
10	BBP	25	0.9988	62.23	9.19
11	BBEP	25	0.99	74.84	8.28
12	DCHP	10	0.992	75.12	12.48
13	DEHP	10	0.9917	119.36	3.47
14	DNOP	10	0.994	64.53	5.75
15	DNP	25	0.991	63.16	13.05
Es and BPA					
1	Diethylestradiol	5	0.996	71.92	4.69
2	Estrone	10	0.992	78.39	7.19
3	17- β -estradiol	5	0.997	86.06	10.5
4	17- α -Ethinylestradiol	25	0.998	104.91	12.17
5	Estriol	25	0.995	81.91	2.22
6	Estradiol valerate	5	0.997	100.52	8.42
7	Bisphenol A	10	0.995	61.63	17.03

Note: "MQL" represents "method quantification limit" which was the concentration whose value of signal to noise was 10 (analyzed by the GC-MS).

Table S6 The detail information of compared sites in this study

Sample sites	Compounds	Number	Location of adjacent sites	Longitude	Latitude
A (115.618858°E, 40.229813°N)	PAHs	a	Outlet of Guanting Resvoir	115.3559°E	40.1502°N
	PAEs	b	Outlet of Guanting Resvoir		
		c	Outlet of Guanting Resvoir		
		d	Outlet of Guanting Resvoir		
	DDE	e	Outlet of Guanting Resvoir	115.6025°E	40.2519°N
B (116.462835°E, 40.145276°N)	PAHs	f	Upper reaches of Wenyu River		
	PAEs	h	Beijing section of Beiyun river		
	DDE	i	Upper reaches of Wenyu River	116.5705°E	40.0175°E
	Es	j	Upper reaches of Wenyu River	116.3814°E	40.5914°N
	BPA	j	Upper reaches of Wenyu River	116.3814°E	40.5914°N
D (116.916628°E, 39.77514°N)	PAHs	g	Outflow of Beiyun River		
	PAEs	h	Beijing section of Beiyun river		
	PAHs	k	Beijing section of Beiyun river		

Notes: a Huang et al. (2005); b Wang et al. (2006); c Zheng et al. (2014); d Ma et al. (2001); e Xue et al. (2006); f Luo et al. (2009); g Shen et al. (2009); h Sui et al. (2008); i Luo et al. (2011); j Lei et al. (2008); k Xue et al. (2015)

Table S7 Chronic toxicity data and PNEC value of detected compounds

Compounds	CASN	ChV (mg·L ⁻¹)	PNEC _{water} (μg·L ⁻¹)	KOC (L·kg ⁻¹)	PNEC _{sed} (μg·kg ⁻¹ ,dw)
PAHs(16)					
NAP	91-20-3	1.000	10.000	1837	403.4
ACEY	208-96-8	0.280	2.800	6123	352.968
ACE	83-32-9	0.180	1.800	6123	226.908
FIUO	86-73-7	0.260	2.600	11290	596.44
PHE	85-01-8	0.14	1.400	20830	588.28
AN	120-12-7	0.140	1.400	20400	576.24
FIUOAN	206-44-0	0.052	0.520	70850	738.712
PY	129-00-0	0.052	0.520	69410	723.736
BaAN	56-55-3	0.019	0.190	23130	88.578
CHRY	218-01-9	0.019	0.190	23610	90.402
BbF	205-99-2	0.006	0.060	803100	963.936
BkF	207-08-9	0.006	0.060	786800	944.376
BaPY	50-32-8	0.006	0.060	253500	304.416
DiBAN	53-70-3	0.002	0.020	2622000	1048.872
BPER	191-24-2	0.002	0.020	2676000	1070.472
INDPY	193-39-5	0.002	0.020	1951000	780.472
PAEs(4)					
DMP	131-11-3	3.300	33.000	251.59	284.8494
DEP	84-66-2	0.820	8.200	714.85	146.7554
DIBP	84-69-5	0.061	0.610	5368.3	67.68926
DnBP	84-74-2	0.048	0.480	8405.45	82.42032
OCP(1)					
p,p'-DDE	72-55-9	0.000	0.004	117500	9.64976
Estrogens(4)and Phenol(1)					
BPA	29348	0.550	5.500	37670	4163.5
DES	56-53-1	0.017	0.170	274100	932.552
E1	53-16-7	0.480	4.800	23720	2294.4
E3	50-27-1	1.400	14.000	1209	388.92
E2	57-91-0	0.210	2.100	15350	652.26

Note: "Chv" presents "Chronic Value"; "KOC" presents "Organic chemical absorption constant"