Supplementary Information

Occurrence, spatial and seasonal variations and environmental risk of pharmaceutically active compounds (PhACs) in Pearl River basin, South China

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Fig. S4. Estimated emission and usage (kg/year) of detected PhACs compounds in the Beijiang River (a, b), Xijiang River (c, d), and Maozhou River (e, f).

Fig. S5. The correlation between PhACs-related data and GDP

Text S1 Extraction of PhACs in surface water and sediment samples.

Surface water samples (1 L) were filtered through 0.7 μm glass fiber filters to separate the suspended particulate matter. Each glass fiber filter containing the suspended particulate matter was extracted twice by solvent ultrasonic extraction, the first time with 10 mL methanol and the second time with 5 mL methanol and 5 mL 0.1% formic acid. Each time the sample was vortexed for 20 s, ultrasonicated for 10 min and centrifuged for 5 min at 3000 rpm. The extracted solution was poured into its filtered aqueous sample. The combined samples were spiked with internal standards and extracted by the solid phase extraction (SPE) method. The SPE was performed with 500 mg/6 cc HLB reversed phase cartridges (Waters company, USA) on a 16-position vacuum manifold. The cartridges were preconditioned with 10 mL of methanol and 10 mL Milli-Q water. Then, the sample was extracted at 5 mL/min. After extraction, the cartridges were rinsed with 25 mL of 5% methanol solution twice and were drained for 30 min. The target compounds were successively eluted from each cartridge with 5 mL methanol, 4 mL ethyl acetate and 3 mL dichloromethane. The final extracts were evaporated to dryness under a gentle nitrogen stream and reconstituted with 1 mL methanol.

For acidic and neutral pharmaceuticals, the water samples were extracted according to our previous study (Chen et al., 2010). Waters Oasis HLB cartridges (500 mg, 6 mL) were preconditioned consecutively with 10 mL methanol and 10 mL Milli-Q water before extraction. After the water samples were passed through the cartridges, the cartridges were dried under vacuum for 2 h and then eluted each with 4 × 3 mL of

methanol followed by 3 × 2 mL of dichloromethane. The extracts were concentrated under a gentle stream of nitrogen gas, and then redissolved in 1 mL of methanol.

Internal standards (final concentration: 100 ng/L) were added into the sediment samples (2 g of freeze-dried sludge) and placed into a 4 ℃ refrigerator for 8 h to evaporate the organic reagents. Then the samples were extracted with 10 mL 0.2 M citric acid buffer (pH=3) and 10 mL acetonitrile by vortex for 20 s, ultrasonication for 15 min and centrifugation for 10 min at 3500 rpm. Each supernatant was collected into a 250 mL flat-bottomed flask. The extraction procedure was repeated thrice. After extraction, the supernatants were transferred to a rotary evaporator at 55 ℃ until approximately 15 mL solution left. The condensed sample was diluted with Milli-Q water to 200 mL and added with 0.5 g Na_4EDTA. After that the sample was passed through the SAX-HLB series column (activated with 10 mL methanol and 10 mL Milli-Q water). After loading, the cartridges were rinsed with 25 mL 5% methanol solution twice, followed by 10 mL Milli-Q water to clean up the Na_4EDTA, and then drained for 30 min. The target compounds were eluted from each cartridge with 5 mL methanol for three times. The final extracts were evaporated to dryness under a gentle nitrogen stream and resuspended with 1 mL methanol.

Table S1

Detailed information for the target compounds and internal standards.

Category	Compounds	CAS	Molecular formula	MW	$LogK_{ow}$	pK_a	Internal standards
Anti-inflammatory/analgesics	Salicylic acid	69-72-7	$C_7H_6O_3$	138.1	1.13, 2.26, -2.42	2.3, 3.5	Mecoprop
	Ibuprofen	58560-75-1	$C_{13}H_{18}O_2$	206.3	3.97	4.9	Mecoprop
	Diclofenac	15307-86-5	$C_{14}H_{11}Cl_2NO_2$	296.2	0.70	4.2	Diclofenac-D4
	Fenoprofen	71720-56-4	$C_{30}H_{26}CaO_6$	242.3	3.90	4.5	Fenoprop
	Indometacin	53-86-1	$C_{19}H_{16}ClNO_4$	357.8	4.27	4.5	Fenoprop
	Ketoprofen	22071-15-4	$C_{16}H_{14}O_3$	254.3	3.12	4.5	Fenoprop
	Meclofenamic acid	644-62-2	$C_{14}H_{11}Cl_2NO_2$	296.2	5.12	4.2	Fenoprop
	Mefenamic acid	61-68-7	$C_{15}H_{15}NO_2$	241.3	5.12	4.2	Fenoprop
	Naproxen	22204-53-1	$C_{14}H_{14}O_3$	230.3	3.18	4.2	Fenoprop
	Tolfenamic acid	13710-19-5	$C_{14}H_{12}ClNO_2$	261.7	5.38	4.3	Fenoprop
	Paracetamol	103-90-2	$C_8H_9NO_2$	151.2	0.46	9.4	Dihydrocarbamazepine
Lipid regulators	Clofibric acid	882-09-7	$C_{10}H_{11}ClO_3$	214.7	2.57	3.2	Mecoprop
	Gemfibrozil	25812-30-0	$C_{15}H_{22}O_3$	250.3	4.77	4.7	Fenoprop
Antiepileptic drugs	Carbamazepine	298-46-4	$C_{15}H_{12}N_2O$	236.3	2.45	13.9	Dihydrocarbamazepine
	Primidone	125-33-7	$C_{12}H_{14}N_2O_2$	218.3	0.91		Dihydrocarbamazepine
Antineoplastic drugs	Cyclophosphamide	50-18-0	$C_7H_{15}Cl_2N_2O_2P$	261.1	0.97	2.84	Dihydrocarbamazepine
Psychoactive drug	Fluoxetin	54910-89-3	$C_{17}H_{18}F_3NO$	309.3	4.65		Fluoxetin-d5
	Sertraline	79617-96-2	$C_{17}H_{17}Cl_2N$	306.2	5.29		Dihydrocarbamazepine
	Diazepam	439-14-5	$C_{16}H_{13}ClN_2O$	284.8	2.7	3.4	Diazepam-D_4
	Lorazepam	846-49-1	$C_{15}H_{10}Cl_2N_2O_2$	321.2	2.41	1.3, 11.5	Lorazepam-D_4
	Prazepam	2955-38-6	$C_{19}H_{17}N_2OCl$	324.8	3.99	-	Prazepam-D_5
	Oxazepam	604-75-1	$C_{15}H_{11}ClN_2O_2$	286.7	2.32	-	Oxazepam-D_5
	Alprazolam	28981-97-7	$C_{17}H_{13}ClN_4$	308.8	3.87	-	Alprazolam-D_5
	Temazepam	846-50-4	$C_{16}H_{13}ClN_2O_2$	300.8	2.15	-	Prazepam-D_5
	Nordiazepam	1088-11-5	$C_{15}H_{11}ClN_2O$	270.7	2.87	-	Diazepam-D_4
	Bromazepam	1812-30-2	$C_{14}H_{10}BrN_3O$	316.2	1.93	-	Diazepam-D_4

Category	Compounds	CAS	Molecular formula	MW	$LogK_{ow}$	pK_a	Internal standards
	Chlordiazepoxide	58-25-3	$C_{16}H_{14}ClN_3O$	299.8	2.42	4.80	Diazepam-D_4
	Clonazepam	1622-61-3	$C_{15}H_{10}ClN_3O_3$	315.7	2.53	1.50, 10.50	Lorazepam-D_4
	Flurazepam	17617-23-1	$C_{21}H_{23}ClFN_3O$	387.9	3.02	-	Flurazepam-D_4
	Nitrazepam	146-22-5	$C_{15}H_{11}N_3O_3$	281.3	2.45	-	Diazepam-D_4
	Flunitrazepam	1622-62-4	$C_{16}H_{12}FN_3O_3$	313.3	1.91	-	Flurazepam-D_4
	Clobazam	22316-47-8	$C_{16}H_{13}ClN_2O_2$	300.8	1.82	-	Lorazepam-D_4
	5-CMB	1022-13-5	$C_{14}H_{12}ClNO$	245.7	4.23	-	Diazepam-D_4
	2-ACB	719-59-5	$C_{13}H_{10}ClNO$	231.7	3.69	-	Diazepam-D_4
	6-CPQ	-	$C_{14}H_9ClN_2O$	256.7	-	-	Oxazepam-D_5
	Clozapine	5786-21-0	$C_{18}H_{19}ClN_4$	326.8	2.84	3.70, 7.60	Clozapine-D_4
	Midazolam	59467-70-8	$C_{18}H_{13}ClFN$	325.8	4.33	-	Diazepam-D_4
	Estazolam	29975-16-4	$C_{16}H_{11}ClN_4$	294.8	3.32	-	Estazolam-D_4
Pesticide	Bentazone	25057-89-0	$C_{10}H_{12}N_2O_3S$	240.3	1.67		Fenoprop
	MCPA	94-74-6	$C_9H_9ClO_3$	200.6	2.52		Mecoprop
Internal standards	Dihydrocarbamazepine	3564-73-6	$C_{15}H_{14}N_2O$	238.3	/	/	/
	Mecoprop	7085-19-0	$C_{10}H_{11}ClO_3$	214.6	/	/	/
	Fenoprop	93-72-1	$C_9H_7Cl_3O_3$	269.5	/	/	/
	Fluoxetine-D_5	1173147-79-9	$C_{17}H_{13}D_5F_3NO$	314.4	/	/	/
	Diclofenac-D_4	153466-65-0	$C_{14}H_7Cl_2D_4NO_2$	300.2	/	/	/
	Diazepam-D_4	65854-76-4	$C_{16}H_8D_5ClN_{20}$	289.8	/	/	/
	Lorazepam-D_4	84344-15-0	$C_{15}H_6Cl_2D_4N_2O_2$	325.2	/	/	/
	Prazepam-D_5	152477-89-9	$C_{19}H_{12}ClD_5N_2O$	329.8	/	/	/
	Oxazepam-D_5	65854-78-6	$C_{15}H_6ClD_5N_2O_2$	291.7	/	/	/
	Alprazolam-D_5	125229-61-0	$C_{17}H_8ClD_5N_4$	313.8	/	/	/
	Clozapine-D_4	204395-52-8	$C_{18}D_4H_{15}ClN_4$	330.8	/	/	/
	Flurazepam-D_4	not available	$C_{21}H_{19}D_4ClFN_3O$	391.9	/	/	/
	Estazolam-D_4	170082-16-3	$C_{16}D_5H_6ClN_4$	299.8	/	/	/

MW: Molecular weight (g/mol); 5-CMB：5-Chloro-2-(methylamino)benzophenone; 2-ACB：2-Amino-5-chlorobenzophenone; 6-CPQ：6-Chloro-4-phenyl-2(1H)-quinazolinone.

Table S2

Information of sampling sites from the Beijiang River, Xijiang River, and Maozhou River.

Sampling Sites	Geographic location (N, E)		Sampling time		Flow rate (m/s)	
			Wet season	Dry season	Wet season	Dry season
Maozhou river						
MZR0	22°42′49.26″	113°54′12.38″	June 2018	December 2018	0.3	0.1
MZR1	22°44′20.02″	113°54′29.81″	June 2018	December 2018	1.7	0.3
MZR2	22°46′59.73″	113°54′39.81″	June 2018	December 2018	0.8	0.2
MZR3	22°48′05.91″	113°53′08.05″	June 2018	December 2018	0.7	0.1
MZR4	22°47′38.27″	113°49′33.06″	June 2018	December 2018	0.9	0.2
MZR5	22°45′05.04″	113°46′49.62″	June 2018	December 2018	0.9	0.2
MZR6	22°44′46.85″	113°46′05.67″	June 2018	December 2018	9.1	2.0
Beijiang river						
NR1	24°46'44"	113°13'08"	July 2018	December 2018	47	12
NR2	24°56'58"	113°25'30"	July 2018	December 2018	311	45
NR3	24°51'51"	113°39'46"	July 2018	December 2018	455	63
NR4	24°44'14"	113°32'37"	July 2018	December 2018	827	113
NR5	24°30'37"	113°34'40"	July 2018	December 2018	1173	160
NR6	24°29'02"	113°49'35"	July 2018	December 2018	707	96
NR7	24°27'53"	113°48'34"	July 2018	December 2018	455	62
NR8	24°27'53"	113°48'34"	July 2018	December 2018	455	62
NR9	24°22'02"	113°48'15"	July 2018	December 2018	1712	482
NR10	24°08'38"	113°23'48"	July 2018	December 2018	2800	560
NR11	23°40'59"	113°04'08"	July 2018	December 2018	2689	294
NR12	23°33'58"	112°58'02"	July 2018	December 2018	2821	336
NR13	23°10'30"	112°48'37"	July 2018	December 2018	19945	3318
Xijiang river						
WR1	22°08'32"	110°00'10"	July 2018	December 2018	/	/
WR2	22°12'04"	109°59'09"	July 2018	December 2018	6.24	1.56
WR3	22°12'28"	109°57'15"	July 2018	December 2018	6.24	1.56
WR4	22°40'20"	110°15'20"	July 2018	December 2018	767	40.5
WR5	22°23'08"	110°03'33"	July 2018	December 2018	767	40.5
WR6	22°12'33"	109°52'13"	July 2018	December 2018	767	40.5
WR7	24°30'16"	108°39'41"	July 2018	December 2018	1344	61
WR8	24°16'23"	109°27'29"	July 2018	December 2018	5541	245
WR9	23°29'35"	110°10'43"	July 2018	December 2018	17405	3079
WR10	24°29'02"	111°24'02"	July 2018	December 2018	496	66
WR11	24°18'11"	111°42'56"	July 2018	December 2018	496	66
WR12	23°27'28"	111°26'52"	July 2018	December 2018	20165	3633
WR13	22°49'13"	111°37'29"	July 2018	December 2018	681	84
WR14	22°48'54"	111°40'19"	July 2018	December 2018	681	84
WR15	22°49'07"	111°47'48"	July 2018	December 2018	229	28
WR16	22°56'27"	111°44'17"	July 2018	December 2018	177	55
WR17	23°07'56"	111°49'55"	July 2018	December 2018	487	61
WR18	23°08'26"	111°47'35"	July 2018	December 2018	487	61
WR19	23°08'38"	111°52'20"	July 2018	December 2018	487	61
WR20	22°57'26"	112°06'21"	July 2018	December 2018	229	28
WR21	23°04'28"	112°09'21"	July 2018	December 2018	56302	6958
WR22	23°09'38"	112°35'18"	July 2018	December 2018	22763	3769

Table S3

Method detection limits (MDL) and method quantitative limits (MQL) of analytes in different matrices (n = 3).

Compounds	Surface water		Sediment	
	MDL ($ng \cdot L^{-1}$)	MQL ($ng \cdot L^{-1}$)	MDL ($ng \cdot g^{-1}$)	MQL ($ng \cdot g^{-1}$)
Bentazone	0.054	0.181	0.061	0.203
Clofibric acid	0.060	0.201	0.074	0.248
Diclofenac	0.051	0.169	0.328	1.092
Fenoprofen	0.325	1.082	0.330	1.099
Gemfibrozil	0.038	0.128	0.123	0.411
Ibuprofen	0.466	1.552	0.089	0.297
Indomethacin	0.118	0.393	0.084	0.280
Ketoprofen	0.221	0.736	0.196	0.654
MCPA	0.035	0.116	0.053	0.176
Meclofenamic acid	0.204	0.680	0.875	2.915
Mefenamic acid	0.180	0.599	0.154	0.514
Naproxen	0.196	0.654	0.285	0.951
Salicylic acid	0.267	0.890	0.430	1.433
Tolfenamic acid	0.122	0.405	0.144	0.481
Carbamazepine	0.009	0.029	0.007	0.024
Cyclophosphamide	0.007	0.024	0.007	0.022
Fluoxetin	0.071	0.236	0.215	0.716
Paracetamol	0.070	0.234	0.540	1.798
Primidone	0.031	0.103	0.042	0.138
Sertraline	0.036	0.120	0.012	0.040
Diazepam	0.008	0.028	0.015	0.049
Lorazepam	0.120	0.399	0.043	0.142
Prazepam	0.021	0.072	0.005	0.017
Oxazepam	0.126	0.420	0.038	0.125
Alprazolam	0.029	0.095	0.014	0.047
Temazepam	0.028	0.092	0.009	0.031
Nordiazepam	0.063	0.210	0.010	0.031
Bromazepam	0.037	0.124	0.020	0.066
Chlordiazepoxide	0.166	0.554	0.011	0.038
Clonazepam	0.019	0.063	0.002	0.007
Flurazepam	0.017	0.057	0.012	0.039
Nitrazepam	0.041	0.135	0.012	0.039
Flunitrazepam	0.031	0.102	0.022	0.074
Clobazam	0.026	0.088	0.014	0.046
5-CMB	0.038	0.126	0.015	0.049
2-ACB	0.082	0.273	0.046	0.152
6-CPQ	0.149	0.496	0.110	0.365
Clozapine	0.009	0.031	0.006	0.019
Midazolam	0.018	0.059	0.007	0.024
Estazolam	0.035	0.118	0.019	0.063

5-CMB：5-Chloro-2-(methylamino)benzophenone；2-ACB：2-Amino-5-chlorobenzophenone；6-CPQ：6-Chloro-4-phenyl-2(1H)-quinazolinone.

Table S4

The wastewater treatment capacity and Gross Domestic Product of the counties/districts where sampling sites are located in.

Sampling Sites	Area	Waste water discharge (10,000 tons/year)	Wastewater treatment capacity (10,000 tons/year)	Gross Domestic Product (GDP) (10,000 yuan)
Maozhou river				
MZR0				
MZR1				
MZR2	Baoan District, Shenzhen city, Guangdong Province	34345	33315	36132180
MZR3				
MZR4				
MZR5				
Beijiang river				
NR1	Ruyuan Yao Autonomous County, Shaoguan City, Guangdong Province	1488	1394	826542
NR2	Ruyuan Yao Autonomous County, Shaoguan City, Guangdong Province	1488	1394	826542
NR3	Renhua County, Shaoguan City, Guangdong Province	1880	1761	1089933
NR4	Qujiang District, Shaoguan City, Guangdong Province	5761	5395	1792694
NR5	Qujiang District, Shaoguan City, Guangdong Province	5761	5395	1792694
NR6	Wengyuan County, Shaoguan City, Guangdong Province	1137	1064	91765
NR7	Wengyuan County, Shaoguan City, Guangdong Province	1137	1064	91765
NR8	Wengyuan County, Shaoguan City, Guangdong Province	1137	1064	91765
NR9	Yingde City, Qingyuan City, Guangdong Province	5107	4632	2720263
NR10	Yingde City, Qingyuan City, Guangdong Province	5107	4632	2720263
NR11	Qingcheng District, Qingyuan City, Guangdong Province	9750	8843	5044678
NR12	Qingcheng District, Qingyuan City, Guangdong Province	9750	8843	5044678
NR13	Sanshui District, Foshan City, Guangdong Province	12100	11685	11509091
Xijiang river				
WR1	Bobai County, Yulin City, Guangxi Zhuang Autonomous Region	3180	2989	2459647
WR2	Bobai County, Yulin City, Guangxi Zhuang Autonomous Region	3180	2989	2459647
WR3	Bobai County, Yulin City, Guangxi Zhuang Autonomous Region	3180	2989	2459647
WR4	Bobai County, Yulin City, Guangxi Zhuang Autonomous Region	3180	2989	2459647
WR5	Bobai County, Yulin City, Guangxi Zhuang Autonomous Region	3180	2989	2459647
WR6	Bobai County, Yulin City, Guangxi Zhuang Autonomous Region	3180	2989	2459647

Sampling Sites	Area	Waste water discharge (10,000 tons/year)	Wastewater treatment capacity (10,000 tons/year)	Gross Domestic Product (GDP) (10,000 yuan)
WR7	Yizhou District, Hechi City, Guangxi Zhuang Autonomous Region	1652	1140	1132160
WR8	Yufeng District, Liuzhou City, Guangxi Zhuang Autonomous Region	1153	1153	5437653
WR9	Guiping City, Guigang City, Guangxi Zhuang Autonomous Region	2382	2082	3156863
WR10	Pinggui District, Hezhou City, Guangxi Zhuang Autonomous Region	3548	3304	1365266
WR11	Babu District, Hezhou City, Guangxi Zhuang Autonomous Region	5677	5286	2118226
WR12	Fengkai County, Zhaoqing City, Guangdong Province	2000	1991	1637100
WR13	Luoding City, Yunfu City, Guangdong Province	2786	2618	2422771
WR14	Luoding City, Yunfu City, Guangdong Province	2786	2618	2422771
WR15	Yunan District, Yunfu City, Guangdong Province	362	340	941064
WR16	Yunan County, Yunfu City, Guangdong Province	1051	987	1071150
WR17	Deqing County, Zhaoqing City, Guangdong Province	2300	2289	1336800
WR18	Deqing County, Zhaoqing City, Guangdong Province	2300	2289	1336800
WR19	Deqing County, Zhaoqing City, Guangdong Province	2300	2289	1336800
WR20	Yuncheng District, Yunfu City, Guangdong Province	3212	3194	1917824
WR21	Gaoyao District, Zhaoqing City, Guangdong Province	6000	5972	4308380
WR22	Dinghu District, Zhaoqing City, Guangdong Province	2814	2801	1131800

The data come from China Statistical Yearbook and Statistical Yearbook of each city. China Statistical Publishing House, 2018, 2019.

Table S5

Parameters required for back-estimated usage of each compound.

Compound	Excretion rate (%)	Reference	Stability in WW	Reference	Removal rate (%) in WW	Reference
Salicylic acid	/	/	/	/	98.0	Yang et al., 2017
Naproxen	70	(Riva et al., 2015)	/	/	7.6	USEPA EPI
Diclofenac	61	(Riva et al., 2015)	/	/	42.8	Yang et al., 2017
Ibuprofen	12	(Riva et al., 2015)	/	/	88.9	Yang et al., 2017
Gemfibrozil	76	(Huschek et al., 2004)	/	/	31.5	Yang et al., 2017
Carbamazepine	2-3	(Clara et al., 2004; Petrie et al., 2015)	/	/	-9.55	Yang et al., 2017
Paracetamol	54	(Riva et al., 2015)	/	/	99.8	Yang et al., 2017
Diazepam	1	(Smith-Kielland et al., 2001)	-3	(Borova et al., 2014; Castrignanò et al., 2016; Herrero et al., 2015; Kosjek et al., 2012; Racamonde et al., 2014)	-30.7	Lei et al., 2021
Clozapine	/	/	/	/	22.8	Lei et al., 2021
Nordiazepam	~7		15.6	(Baker et al., 2014; Borova et al., 2014; Castrignanò et al., 2016; Racamonde et al., 2014)	25.4	Lei et al., 2021
MCPA	/	/	/	/	8.47	USEPA EPI
Bentazone	/	/	/	/	2.71	USEPA EPI
Indomethacin	/	/	/	/	43.65	USEPA EPI
Mefenamic acid	/	/	/	/	81.16	USEPA EPI
Cyclophosphamide	/	/	/	/	1.86	USEPA EPI
Sertraline	/	/	/	/	84.99	USEPA EPI

WW: wastewater; USEPA EPI: USEPA EPI Suite™-Estimation Program Interface.

Table S6

Comparison of PhACs concentrations in surface waters among different area in China.

Compounds	Concentrations (ng/L)	Research area	Reference
Diclofenac acid	< MQL - 53.9 (6.78)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 58 (14.5)	Wujin District, Changzhou city	Duan et al., 2021
	1.8 - 121.6	Beiyun River, Beijing	Ma et al., 2017
	0 - 986.5 (31.9)	Beiyun River, Beijing	Meng et al., 2022
	ND - 32	Xiangjiang River, Hunan Province	Lin et al., 2018
	ND – 180 (8.7)	China, nationwide	Yao et al., 2018
	0.81 - 11	Jiulong River, Fujian Province	Sun et al., 2016
	1.8 – 1300 (408.2)	Hai River, urban area in Beiyun River, Beijing	Yang et al., 2017
	ND - 31.3	Liuxi River and Zhujiang River, Guangzhou City	Yang et al., 2017
	ND - 45.3	Dongjiang River, Guangdong City	Yang et al., 2018
	ND - 506.92 (22.65)	the northwest of Tai Lake Basin, China	An et al., 2022
Mefenamic acid	1.02 - 4.56 (2.26)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 237 (17.7)	Wujin District, Changzhou city	Duan et al., 2021
	2.0 - 7.3	Beiyun River, Beijing	Ma et al., 2017
	ND - 3.9	Xiangjiang River, Hunan Province	Lin et al., 2018
	ND - 3.14	Jiulong River, Fujian Province	Sun et al., 2016
	ND - 31.3	Hai River, urban area in Beiyun River, Beijing	Yang et al., 2017
	ND - 50.70 (5.70)	the northwest of Tai Lake Basin, China	An et al., 2022
Gemfibrozil	< MQL - 12.4 (2.07)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 2 (0.1)	Wujin District, Changzhou city	Duan et al., 2021
	ND - 8.1	Beiyun River, Beijing	Ma et al., 2017
	0 - 3768.7 (64.0)	Beiyun River, Beijing	Meng et al., 2022
	1.3 / 100 [b]	China, nationwide	Yao et al., 2018
	ND - 0.274	Jiulong River, Fujian Province	Sun et al., 2016
	2.3 - 57.4	Hai River, Urban area in Beiyun River, Beijing	Yang et al., 2017
	ND - 6.71	Dongjiang River, Guangdong City	Yang et al., 2018
	ND	the Pearl River, Guangzhou City	Peng et al., 2008
	ND - 83.43 (0.88)	the northwest of Tai Lake Basin, China	An et al., 2022
Carbamazepine	< MQL - 19.6 (2.43)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 50 (4.4)	Wujin District, Changzhou city	Duan et al., 2021
	10.1 - 199.5	Beiyun River, Beijing	Ma et al., 2017
	0 - 788.7 (56.0)	Beiyun River, Beijing	Meng et al., 2022
	4.9 / 69 [b]	China, nationwide	Yao et al., 2018
	ND - 3.84	Jiulong River, Fujian Province	Sun et al., 2016
	0.2 - 10	Zhujiang River, Guangzhou City	Yang et al., 2013
	0.3 - 5.4	Beijiang River, Guangzhou City	Yang et al., 2013
	20.8 - 772	Hai River, urban area in Beiyun River, Beijing	Yang et al., 2017
	12 / 21.3 [b]	Beijing, China	Wang et al, 2015
	1.5/ 3.2 [b]	Changzhou, China	Wang et al, 2015
	5.8 / 9 [b]	Shenzhen, China	Wang et al, 2015
	ND - 9.15	Liuxi River and Zhujiang River, Guangzhou City	Yang et al., 2017
	ND - 9.78	Dongjiang River, Guangdong City	Yang et al., 2018
	ND - 2.0	the central and lower Yangtze River, China	Wu et al., 2014

	0.3 - 94.1 (15.0)	the Pearl River, Guangzhou City	Yu et al., 2011
	0.08 - 25.28 (5.16)	the northwest of Tai Lake Basin, China	An et al., 2022
Naproxen	< MQL - 28.5 (2.21)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 328	the Pearl River, Guangzhou City	Peng et al., 2008
Clofibric acid	0.43 - 2.74 (1.03)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 9 (1.5)	Wujin District, Changzhou city	Duan et al., 2021
	2.3 - 11.8	Beiyun River, Beijing	Ma et al., 2017
	ND - 4.62	Liuxi River and Zhujiang River, Guangzhou City	Yang et al., 2017
	ND - 248	the Pearl River, Guangzhou City	Peng et al., 2008
	ND - 7.05 (0.60)	the northwest of Tai Lake Basin, China	An et al., 2022
Ibuprofen	< MQL – 289 (25.1)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	9.31 - 128	Liuxi River and Zhujiang River, Guangzhou City	Yang et al., 2017
	ND - 292	Dongjiang River, Guangdong City	Yang et al., 2018
	ND - 99.3	the central and lower Yangtze River, China	Wu et al., 2014
	ND - 1417	the Pearl River, Guangzhou City	Peng et al., 2008
Paracetamol	< MQL - 62.5 (5.34)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	14.8 - 338	Liuxi River and Zhujiang River, Guangzhou City	Yang et al., 2017
	ND - 17.8	Dongjiang River, Guangdong City	Yang et al., 2018
	0 - 339 (Acetaminophen)	Zhujiang River, Guangzhou City	Yang et al., 2013
	27 - 152 (Acetaminophen)	Beijiang River, Guangzhou City	Yang et al., 2013
	ND	the central and lower Yangtze River, China	Wu et al., 2014
	ND - 89.49 (10.14) (Acetaminophen)	the northwest of Tai Lake Basin, China	An et al., 2022
Salicylic acid	6.04 - 160 (19.1)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	12.6 - 6600	Liuxi River and Zhujiang River, Guangzhou City	Yang et al., 2017
	9.75 - 1250	Dongjiang River, Guangdong City	Yang et al., 2018
	9 - 2098	the Pearl River, Guangzhou City	Peng et al., 2008
Indomethacin	< MQL - 4.68 (1.37)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	0 - 52.6 (3.2)	Beiyun River, Beijing	Meng et al., 2022

a min-max (median)

b mean/ max

c min-max (mean)

Table S7

Comparison of PhACs concentrations in surface waters among different area in other countries.

Compounds	Concentrations (ng/L)	Research area/country	Reference
Diclofenac acid	< MQL - 53.9 (6.78)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	1.7 / 3.3	Mainstream of Tone River basin, Japan	NakaDa et al., 2007
	2.6 / 3.3	Tributary of Tone River basin, Japan	NakaDa et al., 2007
	< LOQ - 18740	Spain	Silva et al., 2011; Azzouz et al., 2010; Banjac et al., 2015; Boix et al.,2015; Calderón-Preciado et al., 2011; Collado et al., 2014; Gros et al., 2012, 2007, 2006; Kuster et al., 2008; López-Roldán et al., 2010; López-Serna et al., 2012; Moreno-González et al., 2014; Muñoz et al., 2009; Osorio et al., 2012, 2016; Vazquez-Roig et al., 2012; Mijangos et al., 2018
	1.4 - 33.2	France	Rabiet et al., 2006; Togola and Budzinski, 2008; Vulliet and Cren-Olivé, 2011
	< LOQ - 45.7	Turkey	Aydin and Talinli, 2013
	< 0.5 - 568	UK	Kasprzyk-Hordern et al., 2008a, 2008b, 2009; Ashton et al., 2004
	ND - 675	Italy	Mandaric et al., 2017
	11400 (Maximum concentrations)	Mbokodweni River South of Durban, South Africa	Madikizela and Chimuka, 2016a
Mefenamic acid	1.02 - 4.56 (2.26)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	5 - 36	five rivers in Busan, Korea	Sim et al., 2010
	ND - 9.96	Ebro river basin, Spain	Silva et al., 2011
	< 0.3 - 366	UK	Kasprzyk-Hordern et al., 2008a, 2008b, 2009; Ashton et al., 2004
	2380	Umgeni River, KwaZulu-Natal, South Africa	Gumbi et al., 2017
Gemfibrozil	< MQL - 12.4 (2.07)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 7780	Spain	Silva et al., 2011; Banjac et al., 2015; Boix et al., 2015; Collado et al., 2014; Gros et al., 2012, 2007, 2006; LópezRoldán et al., 2010; López-Serna et al., 2012; Moreno-González et al., 2014; Muñoz et al., 2009; Osorio et al., 2016, 2012
	ND - 2.3	France	Banjac et al., 2015; Togola and Budzinski, 2008
	ND - 790	North America	Boyd et al., 2004; Brun et al., 2006; Kolpin et al., 2002; Metcalfe et al., 2003; Zhang et al., 2007

	ND. - 19.1	Italy	Mandaric et al., 2017
Carbamazepine	ND - 19.6 (2.43)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	4.5 / 12	Mainstream of Tone River basin, Japan	NakaDa et al., 2007
	5.6 / 15	Tributary of Tone River basin, Japan	NakaDa et al., 2007
	12 - 95	five rivers in Busan, Korea	Sim et al., 2010
	ND - 267	Spain	Silva et al., 2011; Azzouz et al., 2010; Banjac et al., 2015; Boix et al., 2015; Calderón-Preciado et al., 2011; Collado et al., 2014; Gros et al., 2012, 2007, 2006; López-Roldán et al., 2010; López-Serna et al., 2012; Moreno-González et al., 2014; Muñoz et al., 2009; Osorio et al., 2016, 2012; Vazquez-Roig et al., 2012; Mijangos et al., 2018
	ND - 6720	France	Comoretto and Chiron, 2005; Feitosa-Felizzola and Chiron, 2009; Rabiet et al., 2006; Togola and Budzinski, 2008; Vulliet and CrenOlivé, 2011
	ND - 137	Italy	Celano et al., 2014; Verlicchi et al., 2014; Mandaric et al., 2017
	< 0.5 - 684	UK	Kasprzyk-Hordern et al., 2008a, 2008b, 2009
	130 - 3240	KwaZulu-Natal, South Africa	Matongo et al., 2015
Naproxen	< MQL - 28.5(2.21)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	12 - 13	five rivers in Busan, Korea	Sim et al., 2010
	ND - 2060	Spain	Silva et al., 2011; Azzouz et al., 2010; Banjac et al., 2015; Boix et al., 2015; Calderón-Preciado et al., 2011; Collado et al., 2014; Gros et al., 2012, 2007, 2006; López-Roldán et al., 2010; López-Serna et al., 2012; Moreno-González et al., 2014; Muñoz et al., 2009; Osorio et al., 2016, 2012
	ND - 9.1	France	Rabiet et al., 2006; Togola and Budzinski, 2008; Vulliet and Cren-Olivé, 2011
	ND - 199	Italy	Celano et al., 2014; Mandaric et al., 2017
	2.6 - 12300	Turkey	Aydin and Talinli, 2013
	< 0.3 - 146	UK	Kasprzyk-Hordern et al., 2008a, 2008b, 2009;
	ND - 4500	North America	Boyd et al., 2004; Brun et al., 2006; Kolpin et al., 2002; Metcalfe et al., 2003; Zhang et al., 2007
	< LOQ - 5340	South and North of the city in Durban	Madikizela and Chimuka, 2016b

	0.43 - 2.74 (1.03)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	4.1 / 7.0	Mainstream of Tone River basin, Japan	NakaDa et al., 2007
	4.2 / 21	Tributary of Tone River basin, Japan	NakaDa et al., 2007
	3 - 14	five rivers in Busan, Korea	Sim et al., 2010
Clofibric acid	ND - 2280	Spain	Silva et al., 2011; Azzouz et al., 2010; Calderón-Preciado et al., 2011; Gros et al., 2007, 2006; Kuster et al., 2008; López-Roldán et al., 2010; López-Serna et al., 2012; Muñoz et al., 2009; Osorio et al., 2012; Mijangos et al., 2018
	ND - 6	Italy	Calamari et al., 2003
	< 0.3 - 164	UK	Kasprzyk-Hordern et al., 2008a, 2008b, 2009
	3.2 - 26.7	North America	Boyd et al., 2004; Brun et al., 2006; Kolpin et al., 2002; Metcalfe et al., 2003; Zhang et al., 2007
	< MQL - 289(25.1)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	< LOQ	Mainstream and tributary of Tone River basin, Japan	NakaDa et al., 2007
	29 - 51	five rivers in Busan, Korea	Sim et al., 2010
	< LOQ - 9890	Spain	Silva et al., 2011; Azzouz et al., 2010; Banjac et al., 2015; Calderón-Preciado et al., 2011; Collado et al., 2014; Gros et al., 2012, 2007, 2006; Kuster et al., 2008; López-Roldán et al., 2010; Muñoz et al., 2009; Osorio et al., 2016, 2012; Vazquez-Roig et al., 2012
Ibuprofen	< LOQ - 5.5	France	Rabiet et al., 2006; Togola and Budzinski, 2008; Vulliet and Cren-Olivé, 2011
	< LOQ - 240	Italy	Calamari et al., 2003; Celano et al., 2014; Mandaric et al., 2017
	< LOQ - 263	Turkey	Aydin and Talinli, 2013
	< 0.3 - 5044	UK	Kasprzyk-Hordern et al., 2008a, 2008b, 2009; Roberts et al., 2006; Ashton et al., 2004
	ND - 6400	North America	Boyd et al., 2004; Brun et al., 2006; Kolpin et al., 2002; Metcalfe et al., 2003; Zhang et al., 2007
	8.46×10^4 (max)	KwaZulu-Natal, South Africa	Matongo et al., 2015
	< MQL - 62.5(5.34)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	acetaminophen: 22 / 52	Mainstream of Tone River basin, Japan	NakaDa et al., 2007
Paracetamol	acetaminophen: 18 / 110	Tributary of Tone River basin, Japan	NakaDa et al., 2007
	acetaminophen: 18 - 76	five rivers in Busan, Korea	Sim et al., 2010
	acetaminophen: ND - 9606	Spain	Silva et al., 2011; Banjac et al., 2015; Boix et al.,

			2015; Calderón-Preciado et al., 2011; Collado et al., 2014; Gros et al., 2012, 2006; López-Roldán et al., 2010; López-Serna et al., 2012; Moreno-González et al., 2014; Muñoz et al., 2009; Osorio et al., 2016, 2012; Vazquez-Roig et al., 2012; Mijangos et al., 2018
	ND - 72.3	France	Rabiet et al., 2006; Togola and Budzinski, 2008; Vulliet and Cren-Olivé, 2011
	acetaminophen: < 1.5 - 2382	UK	Kasprzyk-Hordern et al., 2008a, 2008b, 2009
	990 - 1740	KwaZulu-Natal, South Africa	Matongo et al., 2015
	acetaminophen: ND - 226	Adige River, Italy	Mandaric et al., 2017
Salicylic acid	6.04 – 160 (19.1)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 89	Spain	Collado et al., 2014; Groset al., 2012; López-Serna et al., 2012; Moreno-González et al., 2014
	6.7	France	Vulliet and Cren-Olivé, 2011
	< 0.3 - 302	UK	Kasprzyk-Hordern et al., 2008a, 2008b, 2009
	15 - 1700	North America	Boyd et al., 2004; Brun et al., 2006; Kolpin et al., 2002; Metcalfe et al., 2003; Zhang et al., 2007
	4.57 - 190	Adige River, Italy	Mandaric et al., 2017
Indomethacin	< MQL - 4.68 (1.37)	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	16 / 16	Mainstream of Tone River basin, Japan	NakaDa et al., 2007
	6.3 / 8.7	Tributary of Tone River basin, Japan	NakaDa et al., 2007
	ND - 62.5	Ebro river basin, Spain	Silva et al., 2011
	ND - 28.5	Adige River, Italy	Mandaric et al., 2017
Ketoprofen	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	24 / 24	Mainstream of Tone River basin, Japan	NakaDa et al., 2007
	< LOQ	Tributary of Tone River basin, Japan	NakaDa et al., 2007
	ND - 1060	Spain	Silva et al., 2011; Mijangos et al., 2018
	< 0.5 - 14	UK	Kasprzyk-Hordern et al., 2008a, 2008b, 2009
	ND - 193	Adige River, Italy	Mandaric et al., 2017
Diazepam	0.03 - 25.0	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 2.68	Ebro river basin, Spain	Silva et al., 2011
Clozapine	< MQL - 5.83	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	2180 - 8890	KwaZulu-Natal, South Africa	Matongo et al., 2015
Lorazepam	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 46.1	Ebro river basin, Spain	Silva et al., 2011

	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
Fluoxetine	ND - 54	Spain	Banjac et al., 2015; Gros et al., 2012, 2006; López-Roldán et al., 2010; López-Serna et al., 2012; Moreno-González et al., 2014; Muñoz et al., 2009; Osorio et al., 2016, 2012

a min-max (median)

b mean/ max

c min-max (mean)

Table S8

Comparison of concentrations in sediments among different area.

Compounds	Concentrations (ng/g)	Research area	Reference
Diclofenac acid	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	< LOQ - 3.36	Ebro river basin, Spain	Silva et al., 2011
	4.96 - 11.02	Guadalete River basin, Spain	Biel-Maeso et al., 2017
Mefenamic acid	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 12.4	Ebro river basin, Spain	Silva et al., 2011
	1.60 - 3.34	Guadalete River basin, Spain	Biel-Maeso et al., 2017
Gemfibrozil	< MQL - 19.2	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 3.49	Ebro river basin, Spain	Silva et al., 2011
	< LOQ - 0.39	Guadalete River basin, Spain	Biel-Maeso et al., 2017
Carbamazepine	< MQL - 0.61	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 2.84	Ebro river basin, Spain	Silva et al., 2011
	< LOQ - 6.07	KwaZulu-Natal, South Africa	Matongo et al., 2015
	0.07 - 0.76	Guadalete River basin, Spain	Biel-Maeso et al., 2017
Naproxen	< MQL - 8.58	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 1.87	Ebro river basin, Spain	Silva et al., 2011
Clofibric acid	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 56.8	Ebro river basin, Spain	Silva et al., 2011
Ibuprofen	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 20.9	Ebro river basin, Spain	Silva et al., 2011
	< LOQ - 659	KwaZulu-Natal, South Africa	Matongo et al., 2015
	5.83 - 24.93	Guadalete River basin, Spain	Biel-Maeso et al., 2017
	ND - 2.044	Adige River, Italy	Mandaric et al., 2017
Paracetamol	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	acetaminophen: ND - 222	Ebro river basin, Spain	Silva et al., 2011
	acetaminophen: < LOQ - 15.8	KwaZulu-Natal, South Africa	Matongo et al., 2015
	acetaminophen: ND - 1.85	Adige River, Italy	Mandaric et al., 2017
Salicylic acid	1.87 - 63.2	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
Indomethacin	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	4.05 - 8.99	Guadalete River basin, Spain	Biel-Maeso et al., 2017
Ketoprofen	ND	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	ND - 3.34	Ebro river basin, Spain	Silva et al., 2011
Clozapine	< MQL - 3.28	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
	< LOQ - 17.89	KwaZulu-Natal, South Africa	Matongo et al., 2015
Diazepam	< MQL - 2.46	Beijiang, Xijiang and Maozhou River, the Pearl River	this study
Sertraline	0.08 - 0.23	Beijiang, Xijiang and Maozhou River, the Pearl River	this study

a min-max (median)

b mean/ max

c min-max (mean)

Table S9

Spearman's correlations of the concentrations of PhACs between in surface waters and sediments of the Pearl River.

Compounds	Spearman's correlations between in surface waters and sediments
Salicylic acid	**0.027***
Gemfibrozil	0.427
Naproxen	0.562
Clozapine	**0.002****
Diazepam	**< 0.001****
Carbamazepine	**< 0.001****

significant correlations in bold, * $p < 0.05$, ** $p < 0.01$.

Fig. S1

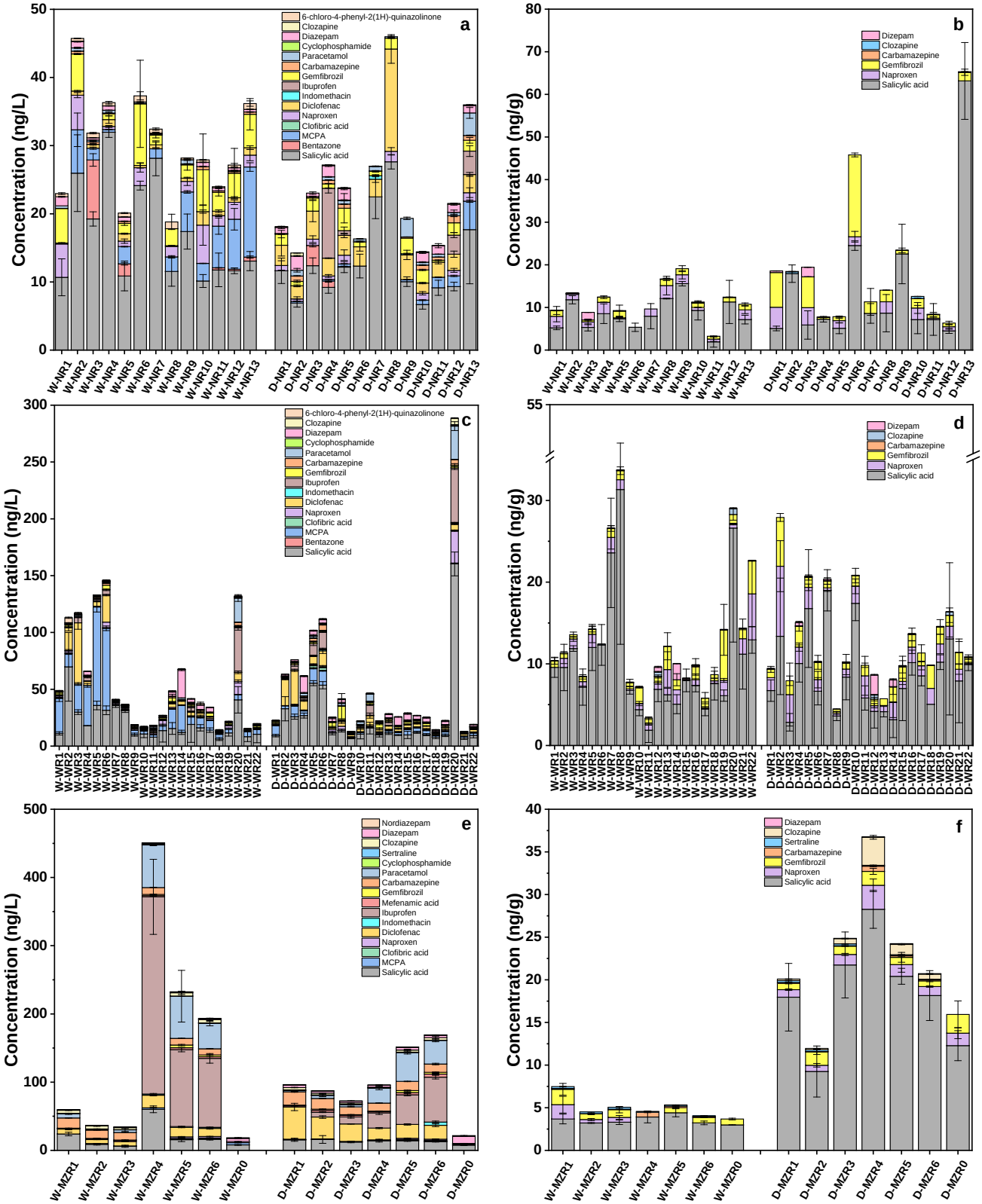

a
Concentration (ng/L)
6-chloro-4-phenyl-2(1H)-quinazolinone
Clozapine
Diazepam
Cyclophosphamide
Paracetamol
Carbamazepine
Gemfibrozil
Ibuprofen
Indomethacin
Diclofenac
Naproxen
Clofibric acid
MCPA
Bentazone
Salicylic acid
W-NR1 W-NR2 W-NR3 W-NR4 W-NR5 W-NR6 W-NR7 W-NR8 W-NR9 W-NR10 W-NR11 W-NR12 W-NR13
D-NR1 D-NR2 D-NR3 D-NR4 D-NR5 D-NR6 D-NR7 D-NR8 D-NR9 D-NR10 D-NR11 D-NR12 D-NR13
b
Concentration (ng/g)
Dizepam
Clozapine
Carbamazepine
Gemfibrozil
Naproxen
Salicylic acid
c
Concentration (ng/L)
d
Concentration (ng/g)
e
Concentration (ng/L)
Nordiazepam
Diazepam
Clozapine
Sertraline
Cyclophosphamide
Paracetamol
Carbamazepine
Gemfibrozil
Mefenamic acid
Ibuprofen
Indomethacin
Diclofenac
Naproxen
Clofibric acid
MCPA
Salicylic acid
W-MZR1 W-MZR2 W-MZR3 W-MZR4 W-MZR5 W-MZR6 W-MZR0
D-MZR1 D-MZR2 D-MZR3 D-MZR4 D-MZR5 D-MZR6 D-MZR0
f
Concentration (ng/g)
Diazepam
Clozapine
Sertraline
Carbamazepine
Gemfibrozil
Naproxen
Salicylic acid

Fig. S2

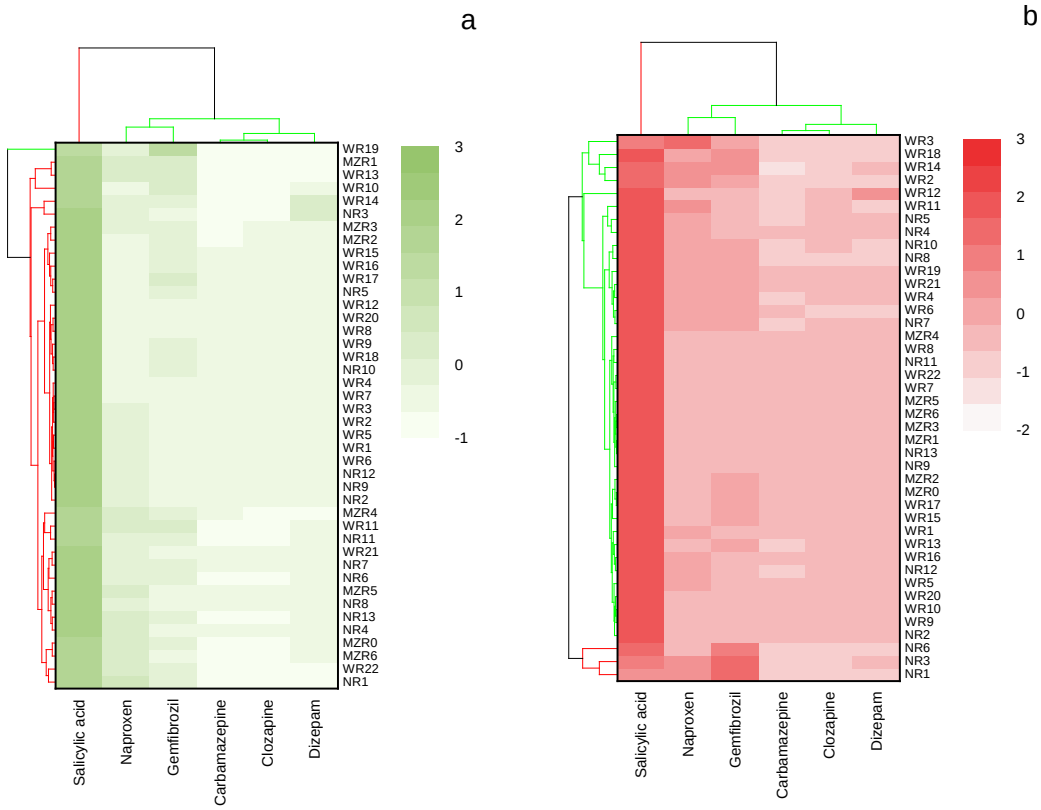

a
WR19
MZR1
WR13
WR10
WR14
NR3
MZR3
MZR2
WR15
WR16
WR17
NR5
WR12
WR20
WR8
WR9
WR18
NR10
WR4
WR7
WR3
WR2
WR5
WR1
WR6
NR12
NR9
NR2
MZR4
WR11
NR11
WR21
NR7
NR6
MZR5
NR8
NR13
NR4
MZR0
MZR6
WR22
NR1
3
2
1
0
-1
Salicylic acid
Naproxen
Gemfibrozil
Carbamazepine
Clozapine
Dizepam
b
WR3
WR18
WR14
WR2
WR12
WR11
NR5
NR4
NR10
NR8
WR19
WR21
WR4
WR6
NR7
MZR4
WR8
NR11
WR22
WR7
MZR5
MZR6
MZR3
MZR1
NR13
NR9
MZR2
MZR0
WR17
WR15
WR1
WR13
WR16
NR12
WR5
WR20
WR10
WR9
NR2
NR6
NR3
NR1
3
2
1
0
-1
-2
Salicylic acid
Naproxen
Gemfibrozil
Carbamazepine
Clozapine
Dizepam

Fig. S3

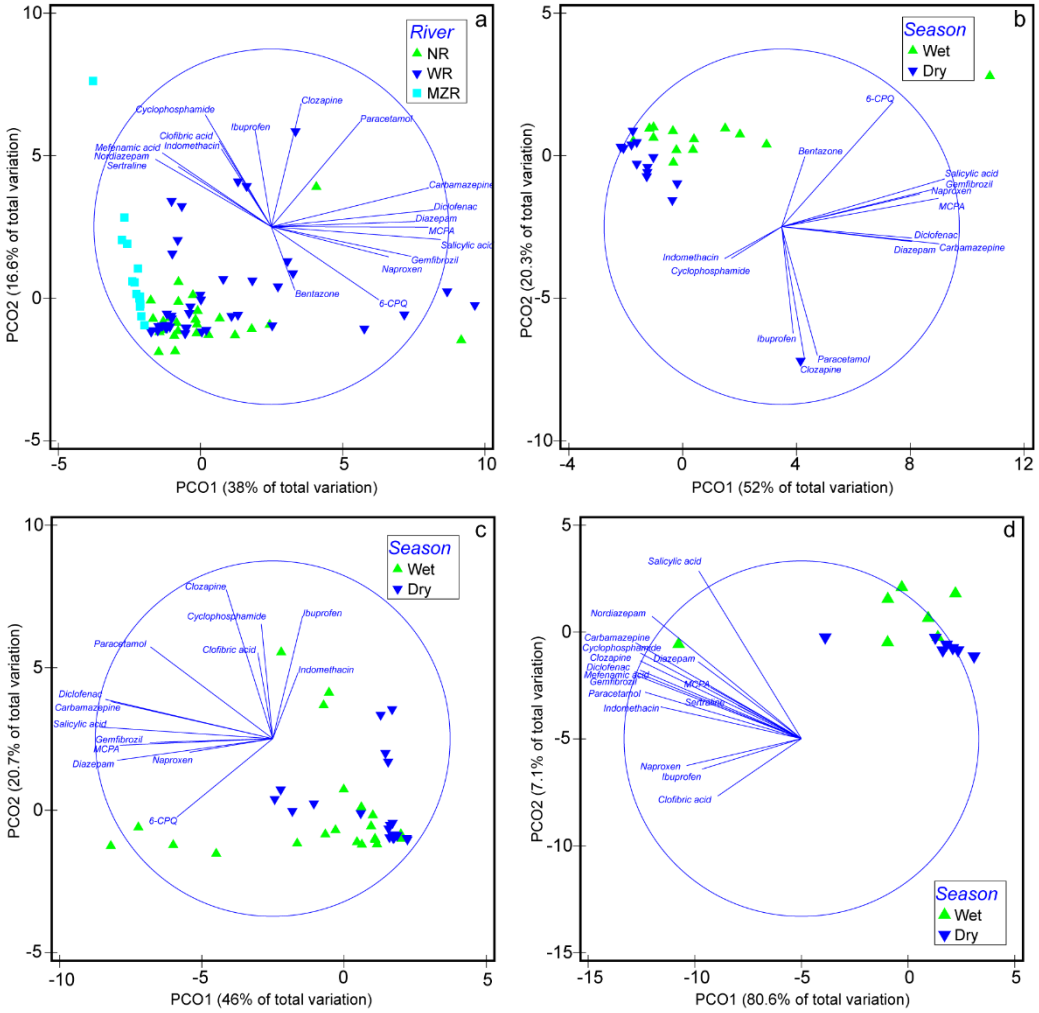

a
River
NR
WR
MZR
Cyclophosphamide
Clofibric acid
Ibuprofen
Clozapine
Paracetamol
Mefenamic acid
Indomethacin
Nordiazepam
Sertraline
Carbamazepine
Diclofenac
Diazepam
MCPA
Salicylic acid
Gemfibrozil
Naproxen
Bentazone
6-CPQ
PCO2 (16.6% of total variation)
PCO1 (38% of total variation)
b
Season
Wet
Dry
6-CPQ
Bentazone
Salicylic acid
Gemfibrozil
Naproxen
MCPA
Diclofenac
Diazepam
Carbamazepine
Indomethacin
Cyclophosphamide
Ibuprofen
Paracetamol
Clozapine
PCO2 (20.3% of total variation)
PCO1 (52% of total variation)
c
Season
Wet
Dry
Clozapine
Cyclophosphamide
Ibuprofen
Paracetamol
Clofibric acid
Indomethacin
Diclofenac
Carbamazepine
Salicylic acid
Gemfibrozil
MCPA
Diazepam
Naproxen
6-CPQ
PCO2 (20.7% of total variation)
PCO1 (46% of total variation)
d
Salicylic acid
Nordiazepam
Carbamazepine
Cyclophosphamide
Clozapine
Diazepam
Diclofenac
Mefenamic acid
Gemfibrozil
MCPA
Paracetamol
Sertraline
Indomethacin
Naproxen
Ibuprofen
Clofibric acid
Season
Wet
Dry
PCO2 (7.1% of total variation)
PCO1 (80.6% of total variation)

Fig. S4

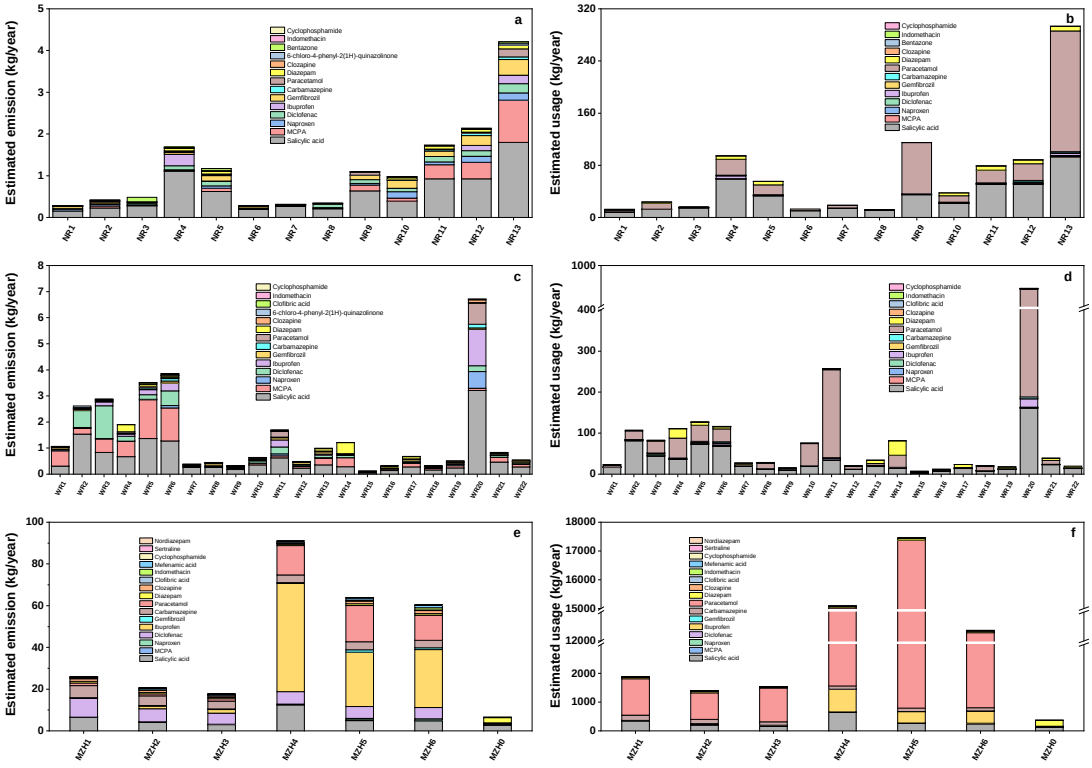
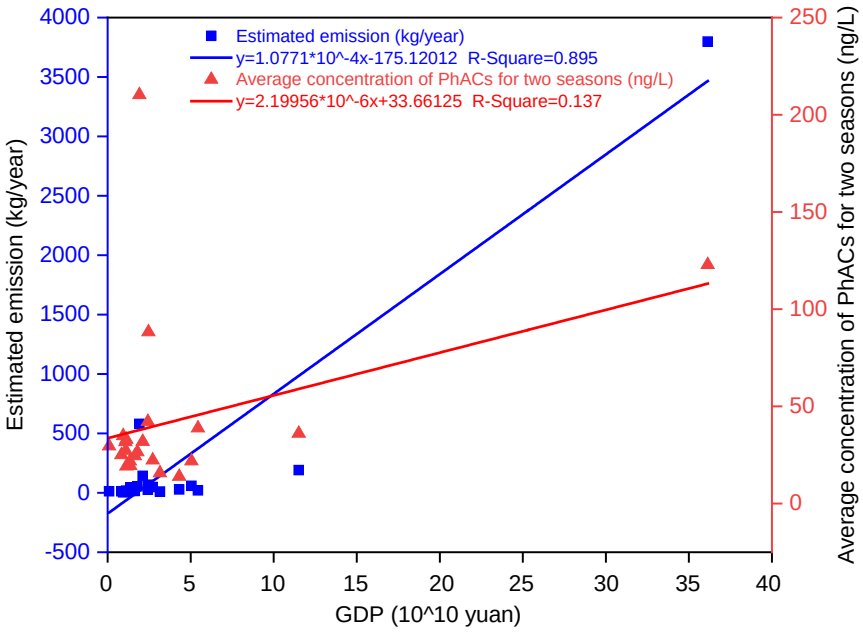

a
Estimated emission (kg/year)
Cyclophosphamide
Indomethacin
Bentazone
6-chloro-4-phenyl-2(1H)-quinazolinone
Clozapine
Diazepam
Paracetamol
Carbamazepine
Gemfibrozil
Ibuprofen
Diclofenac
Naproxen
MCPA
Salicylic acid
NR1 NR2 NR3 NR4 NR5 NR6 NR7 NR8 NR9 NR10 NR11 NR12 NR13
b
Estimated usage (kg/year)
c
Estimated emission (kg/year)
Clofibric acid
WR1 WR2 WR3 WR4 WR5 WR6 WR7 WR8 WR9 WR10 WR11 WR12 WR13 WR14 WR15 WR16 WR17 WR18 WR19 WR20 WR21 WR22
d
Estimated usage (kg/year)
e
Estimated emission (kg/year)
Nordiazepam
Sertraline
Mefenamic acid
MZH1 MZH2 MZH3 MZH4 MZH5 MZH6 MZH7
f
Estimated usage (kg/year)

Fig. S5


Estimated emission (kg/year)
y=1.0771*10^-4x-175.12012 R-Square=0.895
Average concentration of PhACs for two seasons (ng/L)
y=2.19956*10^-6x+33.66125 R-Square=0.137
Estimated emission (kg/year)
Average concentration of PhACs for two seasons (ng/L)
GDP (10^10 yuan)
4000
3500
3000
2500
2000
1500
1000
500
0
-500
250
200
150
100
50
0
0
5
10
15
20
25
30
35
40

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