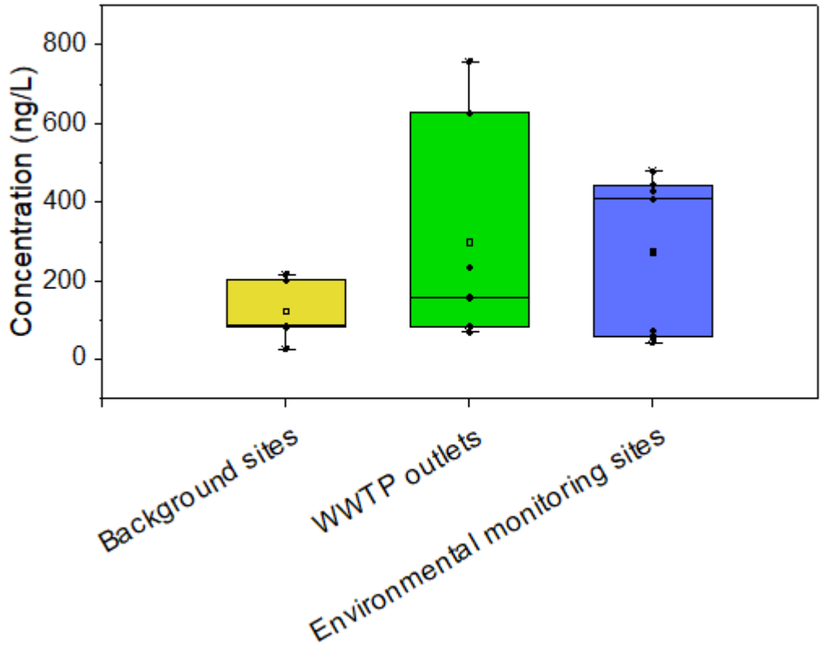

Fig. S1 Cumulative concentrations of PPCPs in different types of sampling sites

Table S1
PPCPs detected in surface water of the Daqing River Basin

Classification		Name	CAS
Antibiotic	Sulfonamide	Sulfadiazine	68-35-9
		Sulfamethazine	57-68-1
		Sulfamethoxazole	723-46-6
		Sulfathiazole	72-14-0
	Fluoroquinolone	Norfloxacin	70458-96-7
		Ofloxacin	82419-36-1
		Ciprofloxacin	85721-33-1
	Tetracycline	Tetracycline	60-54-8
		Oxytetracycline	79-57-2
		Chlortetracycline	57-62-5
	Macrolide	Roxithromycin	80214-83-1
		Erythromycin	114-07-8
		Clarithromycin	81103-11-9
		Lincomycin	154-21-2
		Trimethoprim	738-70-5
Non-antibiotic	Anti-inflammatory	Diclofenac	15307-86-5
		Indomethacin	53-86-1
		Ibuprofen	15687-27-1
		Mefenamic acid	61-68-7
		Naproxen	22204-53-1
	Blood lipid regulator	Bezafibrate	41859-67-0
		Gemfibrozil	25812-30-0
	Anticonvulsant	Carbamazepine	298-46-4
	Disinfectant	Triclosan	3380-34-5

Table S2
Determination and quality control information for PPCPs. Q, quantification transition of different cone and collision voltages; LOD, limit of detection.

Name	ESI mode	Q1	Q2	Retention time (min)	Spiked recoveries (%)	LOD (ng/L)
Sulfadiazine	Positive	251＞156	251＞108	1.11	113	0.20
Sulfamethazine	Positive	279＞186	279＞156	3.70	114	0.50
Norfloxacin	Positive	320＞302	320＞276	3.47	96.0	10.0
Ofloxacin	Positive	362＞318	362＞261	5.10	80.0	10.0
Roxithromycin	Positive	838＞680	838＞158	9.29	64.2	5.00
Sulfamethoxazole	Positive	254＞92	254＞156	1.88	109	0.20
Ciprofloxacin	Positive	332＞288	332＞231	3.76	88.4	10.0
Trimethoprim	Positive	291＞230	291＞123	5.43	120	0.20
Diclofenac	Positive	296＞250	296＞214	7.51	85.0	5.00
Indomethacin	Positive	358＞139	358＞111	7.77	112	1.00
Carbamazepine	Positive	237＞194	237＞179	6.99	113	0.20
Ibuprofen	Negative	224＞207	224＞161	7.41	101	5.00
Bezafibrate	Positive	362＞316	362＞139	6.90	113	0.20
Lincomycin	Positive	407＞359	407＞126	7.35	112	0.20
Erythromycin	Positive	716＞558	716＞158	8.90	95.1	0.20
Clarithromycin	Positive	749＞591	749＞158	9.09	114	0.20

Table S3
Toxicity data of PPCPs

PPCPs	Population	Species	Toxicity data (mg/L)	AF	PNEC (mg/L)
Sulfadiazine	Algae	Selenastrum capricornutum	NOEC = 1	10	0.1
	Crustaceans	Daphnia magna	LOEC = 150	10	15
	Fish	-	LC50 = 907	1000	0.907[a]
Sulfamethazine	Algae	Raphidocelis subcapitata	NOEC = 1	10	0.1
	Crustaceans	Daphnia magna	NOEC = 1.563	10	0.1563
	Fish	Oryzias latipes	NOEC = 10	10	1
Norfloxacin	Algae	Microcystis aeruginosa	NOEC = 0.0016	10	0.00016
	Crustaceans	Daphnia magna	NOEC = 0.12	10	0.012
	Fish	Carassius auratus	NOEC = 0.0027	10	0.00027
Ofloxacin	Algae	-	EC50 = 2440	1000	2.44[a]
	Crustaceans	Daphnia magna	NOEC = 10	10	1
	Fish	Pimephales promelas	NOEC = 10	10	1
Roxithromycin	Algae	Raphidocelis subcapitata	NOEC = 0.01	10	0.001
	Crustaceans	-	LC50 = 6.72	1000	0.00672[a]
	Fish	-	LC50 = 51.6	1000	0.0516[a]
Sulfamethoxazole	Algae	Raphidocelis subcapitata	NOEC = 0.5	10	0.05
	Crustaceans	Daphnia magna	NOEC = 1.11	10	0.111
Diclofenac	Algae	Algae	NOEC = 0.1	10	0.01
	Crustaceans	Daphnia magna	NOEC = 0.00036	10	0.000036
	Fish	Oncorhynchus mykiss	NOEC = 0.00106	10	0.000106
Indomethacin	Algae	Raphidocelis subcapitata	EC50 = 20	1000	0.02
	Crustaceans	Thamnocephalus platyurus	LC50 = 16.14	1000	0.01614
	Fish	Danio rerio	NOEC = 0.001	10	0.0001
Carbamazepine	Algae	Chaetophora sp.	NOEC = 0.002	10	0.0002
	Crustaceans	Daphnia magna	NOEC = 0.0005	10	0.00005
	Fish	Danio rerio	NOEC = 0.01	10	0.001
Ibuprofen	Algae	Selenastrum capricornutum	NOEC = 0.01	10	0.001
	Crustaceans	Daphnia magna	NOEC = 1.23	10	0.123
	Fish	Danio rerio	NOEC = 0.0000664	10	0.00000664
Bezafibrate	Algae	Anabaena sp.	EC50 = 7.62	1000	0.00762
	Crustaceans	Ceriodaphnia dubia	NOEC = 0.023	10	0.0023
	Fish	Danio rerio	NOEC = 0.00003386	10	0.000003386
Lincomycin	Algae	Raphidocelis subcapitata	EC50 = 0.07	1000	0.00007
	Crustaceans	Ceriodaphnia	EC50 = 7.2	1000	0.0072

Ciprofloxacin	Fish	Oryzias latipes	NOEC = 0.5	10	0.05
	Algae	Selenastrum capricornutum	NOEC = 0.5	10	0.05
	Crustaceans	Daphnia magna	EC50 = 1	1000	0.001
	Fish	-	LC50 = 13100	1000	13.1[a]
Trimethoprim	Algae	Anabaena variabilis	NOEC = 3.1	10	0.31
	Crustaceans	Daphnia magna	NOEC = 3.12	10	0.312
	Fish	Danio rerio	NOEC = 0.157	10	0.0157
Erythromycin			dubia		
	Fish	Danio rerio	NOEC = 1000	10	100
	Algae	Synechococcus leopoliensis	NOEC = 0.002	10	0.0002
	Crustaceans	Daphnia magna	NOEC = 11.1	10	1.11
	Fish	Oryzias latipes	NOEC = 100	10	10
Clarithromycin	Algae	Raphidocelis subcapitata	NOEC = 0.04	10	0.004
	Crustaceans	Ceriodaphnia dubia	EC50 = 8.16	1000	0.00816
	Fish	Danio rerio	NOEC = 1000	10	100

[a] The PNEC of PPCPs estimated by ECOSAR (V2.0) if no toxicity data was available.

Table S4
Occurrence of PPCPs in surface water of the Daqing River Basin

Name	Mean of the rank sums	Freq. (%)
Sulfadiazine	136	83.3
Sulfamethazine	112	66.7
Norfloxacin	203	58.3
Ofloxacin	278	91.7
Roxithromycin	188	58.3
Sulfamethoxazole	240	100
Ciprofloxacin	76.3	8.33
Trimethoprim	156	75
Diclofenac	192	58.3
Indomethacin	126	45.8
Carbamazepine	238	100
Ibuprofen	87.9	12.5
Bezafibrate	132	75
Lincomycin	226	100
Erythromycin	277	100
Clarithromycin	154	58.3

Table S5

Comparison of median concentrations (ng L^{-1}) of 16 detectable PPCPs in this study with others

Location	Country	Sulfadiazine	Sulfamethazine	Norfloxacin	Ofloxacin	Roxithromycin	Sulfamethoxazole	Ciprofloxacin	Trimethoprim	References
Daqing River Basin	China	0.4	0.5	21.6	22	10.5	10.4	ND	2	This study
Yangtze River Delta	China	ND -1.31	0.86-2.65	19	ND-19	ND-8.1	7-30	9.5	ND-1.38	[1–5]
Songhua River	China	——	——	——	ND	——	2.5-4.5	ND	——	[6]
Beiyun River	China	50	20	——	——	——	100	——	302	[7,8]
Zhujiang River	China	——	——	——	——	——	——	——	——	[9]
Liao River	China	——	——	ND	ND	6.75	59.8	ND	——	[10]
Jinsha River	China	ND	——	ND	ND	0.68	0.97	ND	——	[11]
Riyadh surface water	Saudi Arabia	——	——	537[a]	393[a]	——	——	——	——	[12]
Yamuna river	India	——	——	——	——	——	184[a]	115[a]	2188[a]	(Mutiyar et al. 2018; Biswas and Vellanki. 2021)
Wadi Shueib	Jordan	——	——	——	——	——	——	——	——	[15]
Apatlaco River	Mexico	——	——	——	——	——	173[a]-642[a]	——	37[a]-72[a]	[16]
Iberian rivers	Spain	——	——	——	0.07-0.98	——	0.16-0.44	0.1-0.78	0.17-6.17	[17]
Surface water of Saitama, Kyoto, Tokushima	Japan	——	——	ND	——	12.5	30.3	ND	ND	[18]

Location	Country	Diclofenac	Indomethacin	Carbamazepine	Ibuprofen	Bezafibrate	Lincomycin	Erythromycin	Clarithromycin	References
Daqing River Basin	China	7.8	ND	11.8	ND	0.8	8.6	24.3	3	This study
Yangtze River Delta	China	4.4	——	0.3-8.22	22	——	ND-10.6	ND-7.3	ND	[1–5]
Songhua River	China	0.8-3	——	——	2.6	——	4-6.8	1.5-3.6	——	[6]
Beiyun River	China	810	58.6	93.1	——	10-83.9	——	715	10	[7,8]
Zhujiang River	China	25.2	2.61	——	58.2	——	——	——	——	[9]
Liao River	China	——	——	——	——	——	——	——	——	[10]
Jinsha River	China	ND	——	——	ND	——	0.42	ND	0.57	[11]
Riyadh surface water	Saudi Arabia	1188[a]	0.08[a]	——	976[a]	——	——	——	——	[12]
Yamuna river	India	18.5[a] -96.1[a]	——	119[a]-412[a]	662[a]	——	——	——	——	[13,14]
Wadi Shueib	Jordan	35	——	240	250	26	——	——	——	[15]
Apatlaco River	Mexico	283[a] -1209[a]	20[a] -212[a]	19[a] -90[a]	231[a] -836[a]	362[a]-1513[a]	——	——	——	[16]
Iberian rivers	Spain	1.02-11.3	0.16-4.83	0.02-8.88	1.94-34.1	0.03-3.02	——	0.22	0.09-0.25	[17]
Surface water of Saitama, Kyoto, Tokushima	Japan	22.1	30.3	12.7	ND	138	ND	14.9	210	[18]

[a] The average concentrations of PPCPs if no median concentration was available. ND, not detected.

8	21.6	1.5	ND	ND	14.4	ND	ND	2.7	10.9	2.8
34.4	ND	19.5	203	17.8	20.3	26	11	45.4	148	33.3
30.9	ND	7.6	52.9	8	25.4	40.5	6.9	23.2	102	23
12.2	ND	3.2	ND	ND	10.6	ND	1	2.9	27.7	ND
96.9	ND	7.9	81.5	2.9	21.1	ND	4.4	6.3	110	14.7
72.1	ND	6.9	9.9	3	14.5	ND	1.9	4.4	67.9	18.9
2.2	ND	ND	ND	ND	0.7	ND	ND	1.2	2.5	ND
19.9	ND	3.3	34.9	4	29.3	ND	ND	11.9	14.1	3.4
2.3	ND	ND	ND	ND	1.9	ND	0.6	4	3.8	ND
10.4	ND	2.3	45.4	3.7	50	ND	1.1	6.5	80.9	10.6
15.8	16.6	3.8	75.2	5.8	64	ND	1.2	5.2	89.4	13.8
2.4	ND	1.6	5	ND	1.8	ND	0.4	17.5	10.8	ND
15.2	ND	3.1	27.9	3	81.4	ND	1.7	9.7	73.6	8.8
18.8	ND	3.1	23.7	5	227	ND	0.7	12.6	52.5	9
8.7	ND	1.1	9.1	1.3	2.7	ND	ND	6.2	5.7	ND
7.3	ND	ND	14.6	1.4	3.5	ND	ND	7.4	9.2	ND
10.5	ND	2.9	9.5	ND	5.5	ND	1.8	22.7	33.4	4.1
5.8	ND	1.6	ND	ND	13	ND	1.2	11.7	20.9	ND
10.3	ND	2.9	ND	ND	2.7	ND	5.8	30.5	70.3	3.3
6.3	ND	ND	ND	ND	3.3	ND	0.6	1.9	6.1	ND
2.6	ND	1.2	ND	ND	2.7	12.5	0.3	0.8	8.8	ND
3.1	ND	ND	ND	ND	3.6	ND	ND	13.5	5.7	ND
10.7	ND	1	ND	ND	16.8	ND	0.6	12.1	50.4	5.4
4.9	ND	ND	6.4	ND	9.5	ND	1.4	23.3	16.6	2.4

Table S7
Concentrations (mg/L) of conventional water pollutants at different sampling site

Sampling site	COD	BOD_5	TP	TN	NH_4-N
JB1	17	1.1	0.06	2.94	0.22
JW1	21	7.6	0.21	5.06	1.58
JE1	25	7.6	0.23	5.07	2.42
JB2	9	1.9	0.05	3.24	0.13
JE2	13	1.7	0.05	4.75	0.22
JE3	9	1.3	0.06	4.78	0.14
FB1	7	1.9	0.02	2.76	0.08
FW1	7	1.5	0.03	2.8	0.34
FE1	7	1.9	0.04	2.33	0.23
FE2	14	3.7	0.09	3.71	0.45
FW2	23	3	0.11	4.26	0.28
FW3	9	2.3	0.06	2.36	0.23
FE3	16	1.7	0.08	4.04	0.27
FE4	15	1.6	0.06	3.33	0.19
XB1	6	1.2	0.02	3.3	0.05
XB2	6	1.4	0.03	3.13	0.02
XW1	14	2.1	0.07	3.43	0.26
XE1	21	2.8	0.1	2.94	0.3
XW2	29	4.1	0.16	2.8	0.59
XE2	11	1.8	0.08	3.38	0.22
XW3	21	2.9	0.08	3.12	0.28
XE3	21	2.6	0.14	1.47	0.19
BL	18	1.9	0.05	1.26	0.23
DR	21	2.3	0.06	1.34	0.44

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