Electronic Supplementary Material (ESI) for Journal of Environmental Monitoring

Supplementary Information

SI1: Pretreatment procedure for sampling

Sampling: Water samples more than 2 L (10 L of pipeline and tap water) were collected using brown glass flasks. Flasks were pre-cleaned three times sequentially using milli-Q water firstly and then acetone before sampling. Approximately 1 g/L of ascorbic acid and 0.5 g/L of EDTA were added into each flask and then dissolved by shaking. During transporting to the lab, the samples were stored in the ice box.

Filtration: 2 L (10 L of pipeline and tap water) water samples were taken using volumetric flasks and then filtered by glass fiber filter papers (1 μm pore size, Whatman GF/B). The filter was washed three times by acetone before filtration.

Solid Phase Extraction (SPE): HLB cartridges (Oasis HLB cartridge, 6cc, Waters) were activated with 6 mL methanol and then with 6 mL milli-Q water by gravity. The HLB equipment (SPC10-C, Sep-Pak concentrator) was purged with methanol and milli-Q water, respectively, each for 5 min at the flow rate of 10 mL/min. HLB cartridges were loaded with water samples. After filtrating water samples, the cartridges were rinsed with milli-Q water three times at the flow rate of 10 mL/min. Finally, the cartridges were purged with methanol and milli-Q water, respectively, each for 5 min at the flow rate of 10 mL/min.

Dewater: The HLB cartridge was dewatered in air for more than two hours.

Elution: PPCPs on the HLB cartridges were eluted with 6 mL methanol by gravity. If the samples would not be analyzed immediately, the elution should be stored at 4 ºC for several days or at –20 ~ -30 ºC for longer time.

Evaporation: The needles of nitrogen evaporator (EYELA MG-2200) were cleaned by acetone. The elute was evaporated using the nitrogen evaporator at 37 ºC and gentle nitrogen flow rate. After evaporation, the needles were cleaned again by acetone.

Dissolution: 1 mL methanol was added into the test tube and the tube was shaken to dissolve PPCPs. If PPCPs could not be dissolved, ultrasonic treatment should be used.

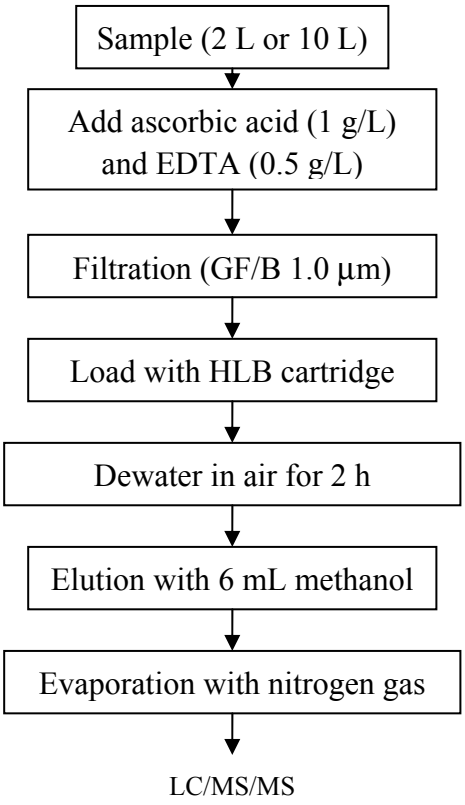

Figure S1 Flow chart for sample pretreatment

SI2: HPLC/MS/MS parameters for 37 PPCPs analysis

Table S1 Apparatus parameters used to analyze 37 PPCPs by LC/MS/MS

No.	PPCPs	Retention time(min)	Ion pair (m/z)
1	Ampicillin	39.1	352/113
2	Azithromycin	45.8	750.2/83
3	Clarithromycin	45.8	749.2/158.1
4	Lincomycin	31.8	408/126
5	Roxithromycin	57.6	838.1/158.1
6	Sulfadimidine	40	280/205.9
7	Sulfamerazine	24	267.1/145
8	Sulfamethoxazole	39.4	254/156
9	Sulfamonomethoxine	46.7	282.9/225
10	Sulfapyridine	31.1	250/156
11	Tiamulin	54	495.1192
12	Trimethoprim	35.8	291/230.2
13	Antipyrine	43.3	189.1/56
14	Caffeine	44.8	195.1/118
15	Diclofenac	42.5	298/201.9
16	Ethenzamide	17	166.1/102.1
17	Indomethacin	33	359.1/126.1
18	Naproxen	55	231.1/189.2
19	Propyphenazone	55	231.1/189.1
20	Atenolol	41.5	268.1/74
21	Metoprolol	41.5	269.1/74.1
22	Salbutamol	21.9	241.1/149.1
23	Bezafibrate	40.5	362/318.1
24	Carbazochrome	53.8	237/194
25	Disopyramide	30.4	342/112.1
26	Ifenprodil	46	327.1/309.2
27	Dipyridamole	54.5	506.1/386.1
28	Carbamazepine	44.9	239.1/194

No.	PPCPs	Retention time(min)	Ion pair (m/z)
29	Primidone	44.8	221.1/193
30	Pirenzepine	39.2	353/113.1
31	Quinoxaline-2-carboxylic acid	48.4	176.1/91
32	Clenbuterol	40	205/132
33	DEET	44.8	194.1/167
34	Crotamiton	40	279/205
35	Diltiazem	51.3	416/178
36	Sulpiride	31.5	342/112.2
37	Theophylline	47.6	183/155.1

SI3: IDLs, MDLs and recoveries of 22 PPCPs

Table S2 IDLs, MDLs and recoveries of 22 PPCPs

No.	PPCPs	CAS	Molecular weight	IDL (ng/L)	MDL (ng/L)	Recovery (%)
1	Ampicillin	7177-48-2	403.45	0.2	0.9	70
2	Azithromycin	83905-01-5	748.99	1.1	3.6	42
3	Clarithromycin	81103-11-9	747.96	1.7	5.5	50
4	Sulfadimizine	57-68-1	278.32	4.8	15.9	66
5	Sulfamerazine	127-79-7	264.30	0.5	1.5	89
6	Sulfamonomethoxine	1220-83-3	280.3	1.8	6.0	65
7	Diclofenac	15307-86-5	278.13	1.12	3.73	77
8	Ethenzamide	938-73-8	165.19	1.3	4.4	60
9	Naproxen	22204-53-1	230.26	0.2	0.7	88
10	Propyphenazone	479-92-5	230.3	0.3	0.8	87
11	Metoprolol	37350-58-6	267.36	1.2	3.9	75
12	Salbutamol	34391-04-3	239.31	4.2	14.1	70
13	Ifenprodil	23210-56-2	325.44	0.4	1.2	50
14	Dipyridamole	58-32-2	504.63	1.2	3.0	81
15	Primidone	125-33-7	218.25	5.4	17.9	106
16	Pirenzepine	28797-61-7	351.4	0.93	3.11	66
17	Quinoxaline-2-carboxylic acid	1196-57-2	146.15	0.54	1.23	70
18	Bezafibrate	41859-67-0	361.82	2.78	8.34	90
19	Clenbuterol	37148-27-9	277.19	0.4	1.3	84
20	Crotamiton	483-63-6	203.28	0.4	2.7	80
21	Diltiazem	42399-41-7	414.52	0.2	0.6	37
22	Theophylline	58-55-9	182.18	2.2	7.3	80