Supplementary Information

Determination of 38 pharmaceuticals and personal care products in water by lyophilization combined with Liquid Chromatography-Tandem Mass Spectrometry

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Table S1: Octanol/water partition coefficients and acid dissociation constants of targeted PPCPs.

Serial no.	Group	CECs	CEC concentration factor in working standard solution	$logK_{ow}$[a]	pKa[a]
1	Antibiotics	Ciprofloxacin	2	-0.81	5.76
2	Antibiotics	Enoxacin	2	-0.98	5.5
3	Antibiotics	Lomefloxacin	1	-0.39	5.64
4	Antibiotics	Levofloxacin	1	0.65	5.45
5	Antibiotics	Metronidazole	1	-0.46	15.44
6	Antibiotics	Norfloxacin	1	-0.92	5.77
7	Antibiotics	Sarafloxacin	1	0.56	5.74
8	Antibiotics	Flumequine	2	2.42	6
9	Antibiotics	Sulfachloropyridazine	1	0.85	6.6
10	Antibiotics	Sulfadiazine	1	0.39	6.99
11	Antibiotics	Sulfadimethoxine	1	1.26	6.91
12	Antibiotics	Sulfameter	1	0.23	7.06
13	Antibiotics	Sulfamethizole	1	0.21	6.71
14	Antibiotics	Sulfamethoxazole	1	0.79	6.16
15	Antibiotics	Sulfapyridine	1	1.01	6.24
16	Antibiotics	Sulfaquinoxaline Na	1	1.55	6.79
17	Antibiotics	Sulfathiazole	1	0.98	6.93
18	Antibiotics	Sulfaguanidine	1	-0.52	10.52
19	Antibiotics	Sulfamerazine	1	0.52	6.99
20	Stimulant	Caffeine	0.25	-0.55	14
21	Stimulant	Cotinine	1	0.34[b]	4.5[b]
22	Antiepileptic agent	Carbamazepine	1	2.77	15.96
23	Adrenergic receptor	Clenbuterol hydrochloride	1	2.33	14.06
24	Nerve agent	Diazepam	1	3.08	-

25	Cardiovascular agent	Sildenafil citrate	1	1.35	10.92
26	Hypoglycemic agent	Glibenclamide	1	3.79	4.32
27	Lipid regulator	Clorfibric acid	1	2.57	-
28	Preservative	Benzylparaben	1	3.40	8.50
29	Preservative	Methylparaben	1	1.67	8.5
30	NSAIDs	Ethenzamide	2	1.61	7.9
31	NSAIDs	Paracetamol	1	0.91	9.46
32	NSAIDs	Mefenamic acid	1	5.40	3.89
33	NSAIDs	Propyphenazone	1	2.35	-
34	Antibacterical agent	Triclocarban	1	4.93	11.42
35	Antifungal agent	Miconazole	1	5.96	-
36	Anti-infective agent	Thiabendazole	1	2.33	10.28
37	Anti-infective agent	Trimethoprim	1	1.28	17.33
38	Anti-infective Agents	Oxolinic acid	1	1.35	5.58

a data are from Drugbank (http://www.drugbank.ca/)
b [1]

1. M. Dobrinas, E. Choong, M. Noetzli, J. Cornuz, N. Ansermot and C. B. Eap, Journal of Chromatography B, 2011, 879, 3574-3582.

Table S2: Sample information including pH, electrical conductivity, total nitrogen (TN), total phosphorus (TP), chemical oxygen demand (COD, wastewater), and total organic carbon (TOC, surface water).

Water samples	pH	Electrical conductivity (μS/cm)	TN (mg/L)	TP (mg/L)	COD/TOC (mg/L)
River	7.2	199	2	0.026	5
Reservoir	8.5	89	2	0.30	6
Influent	7.4	10240	47	3.1	164
Effluent	7.0	1454	17	0.057	24

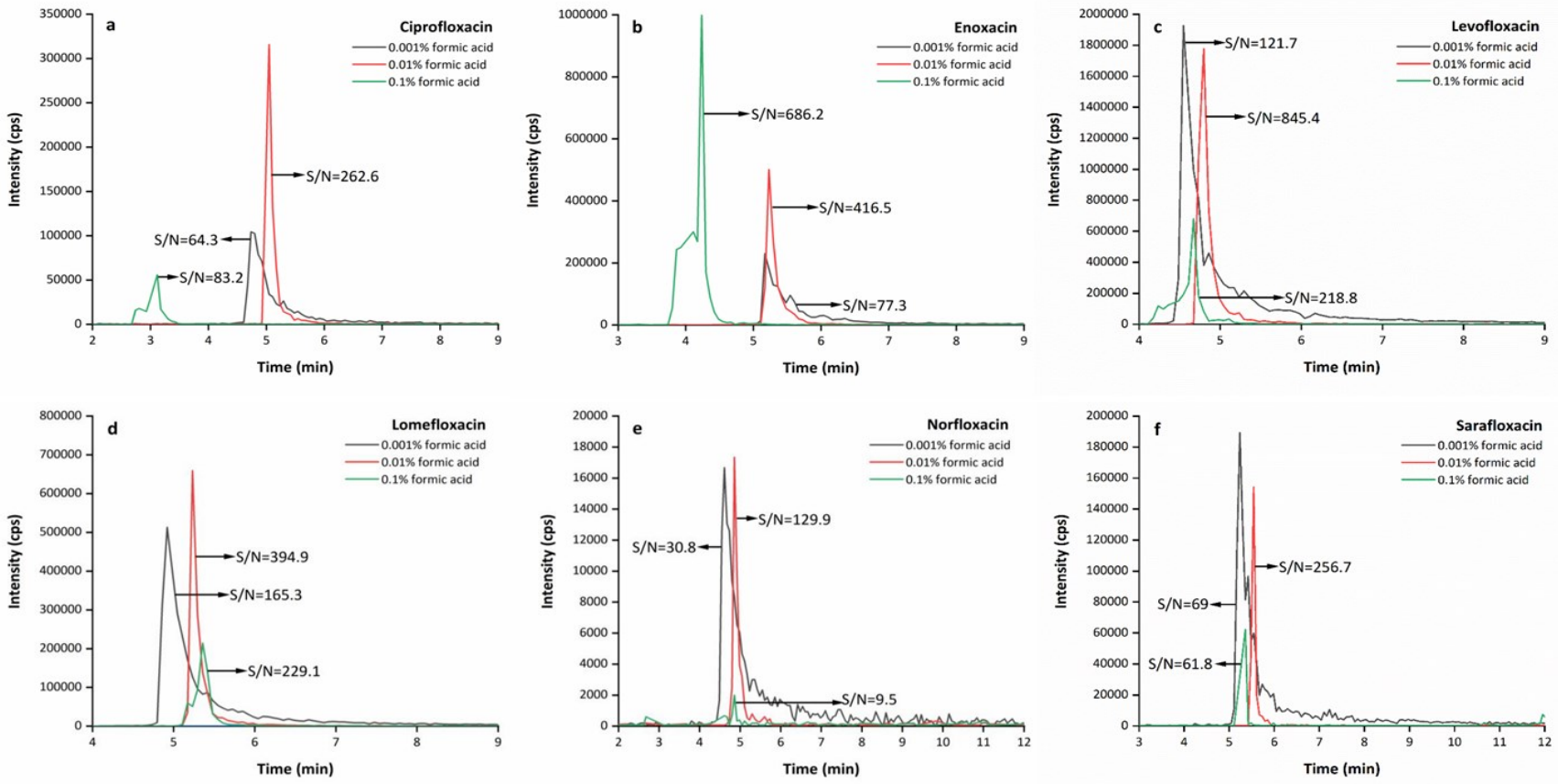

Fig. S1 SRM chromatograms for 6 antibiotics by different concentrations of mobile phase A (a, ciprofloxacin; b, enoxacin; c, levofloxacin; d, lomefloxacin; e, norfloxacin; f, sarafloxacin).