Supplementary Material

Distribution and ecological risk assessment of Pharmaceuticals and personal care products in sediments of North Canal, China

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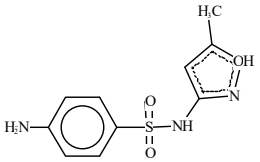
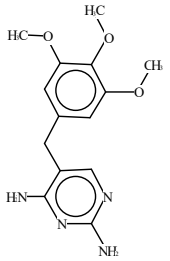
Table S1. Physiochemical properties of the antibiotics considered in the study

PPCPs	Abbreviation	CAS No	Molecular Formula	Structure	MW (g/mol)	Water Solubility (mg/L)	vapor pressure (mm Hg)	$LogK_{ow}$
Sulfamethoxazole	SMX	723-46-6	$C_{10}H_{11}N_3O_3S$		253.28	3942	1.3×10^{-7}	0.89
Trimethoprim	TMP	738-70-5	$C_{14}H_{18}N_4O_3$		290.32	2334	7.52×10^{-9}	0.91

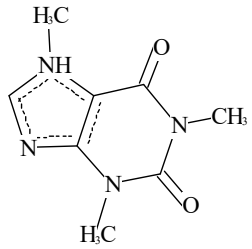
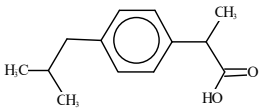
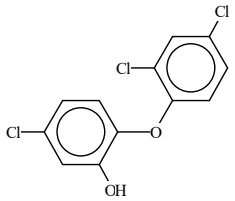
Caffeine	CAF	58-08-2	$C_8H_{10}N_4O_2$		194.19	2632	7.33×10^{-9}	−0.07
Ibuprofen	IBU	15687-27-1	$C_{13}H_{18}O_2$		206.29	41.05	1.86×10^{-4}	3.97
Triclosan	TCS	3380-34-5	$C_{12}H_7CI_3O_2$		289.55	4.621	4.65×10^{-6}	4.76

Table S2 Limit of detection (LOD) and limit of quantification (LOQ) for the the target compounds.

Compounds	Water		Sediment	
	LOD (ng/L)	LOQ (ng/L)	LOD (ng/g)	LOQ (ng/g)
SMX	0.09	0.3	0.05	0.2
TMP	0.01	0.03	0.3	1
CAF	0.2	0.6	0.06	0.2
IBF	1.1	3.3	0.01	0.03
TCS	0.3	0.8	0.1	0.3

[a] The linear range was from 1 to 500 μg/L for all target compounds.

TableS3. Toxicity data used to derivate the predicted no effect concentrations (PNECs) in this study. Bold is the lowest NOEC.

Name	Organisn	Duration	End Pt	Predicted mg/L (ppm)
TMP	Hydra attenuata[1]	96-h	LC50	>100
		96-h	EC50	NC
	Anabaena variabilis NIES-23[2]		EC50	11
	D. magna[3]	48-h	EC50	123
	M. macrocopa[3]	48-h	EC50	54.8
	Dreissena polymorpha[4]	**3-d**	**NOEC**	**0.00029**
SMX	Hydra attenuata[1]	96-h	LC50	>100
	Chlorella vulgaris[1]	48-h	EC50	0.98
	Ceriodaphnia dubia[5]	8-d	NOEC	0.14
	Scenedesmus vacuolatus[6]		EC50	1.54
	Lemna minor[6]		EC50	0.21
	Daphnia magna[7]	48-h	EC50	123.1
	M. macrocopa[7]	48-h	EC50	70.4
	Lemna gibba[8]	**7-d**	**NOEC**	**0.0094**
IBU	Hydra attenuata[1]	96-h	LC50	22.36
		96-h	EC50	1.65
	Daphnia magna[9]	48-h	LC50	132.6
		21-d	NOEC	20
	Oryzias latipes[10]		**NOEC**	**0.00001**
TCS	Chironomus tentans[11]	10-d	LC50	0.4
	Ceriodaphnia dubia[6]	24-h	LC50	0.2
	Pimephales promelas[6]	24-h	LC50	0.36
	Pseudokirchneriella subcapitata[12]	**3-d**	**NOEC**	**0.0002**
CAF	Hydra attenuata[1]	96-h	LC50	>100
	Algae[13]	48-h	EC50	805
	Invertebrate[13]	48-h	EC50	46
	Fish[13]	48-h	EC50	46
	Salmo salar[14]	**5-d**	**NOEC**	**0.0001**

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