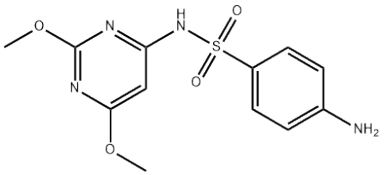
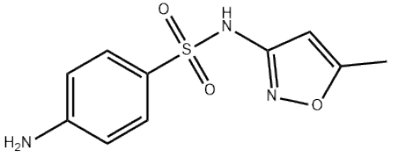
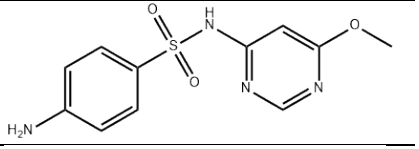
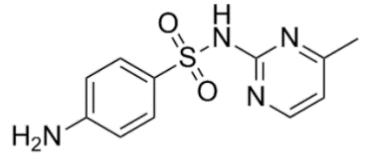
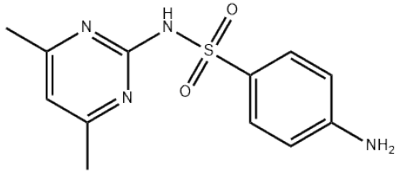
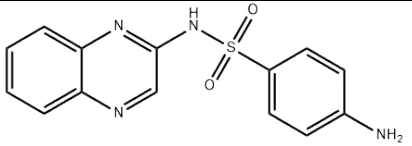
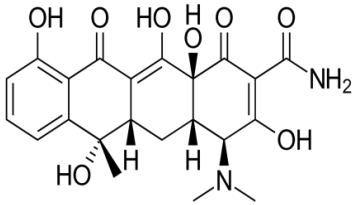
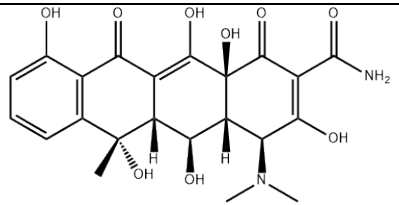
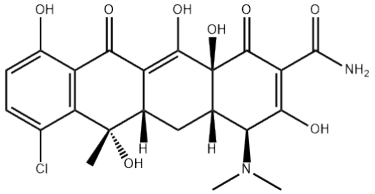
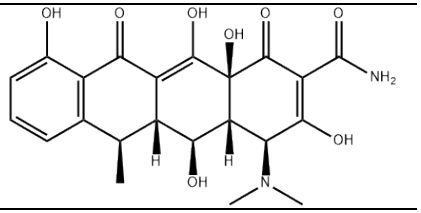
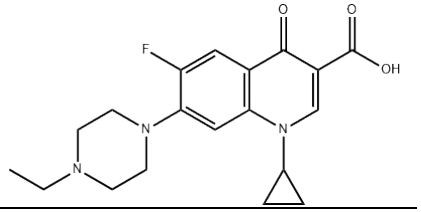
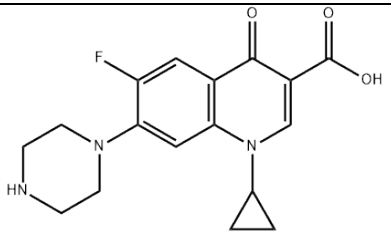
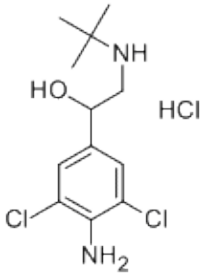
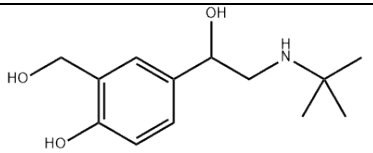
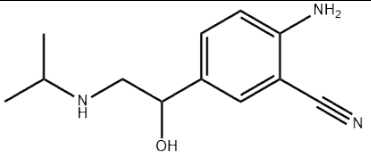
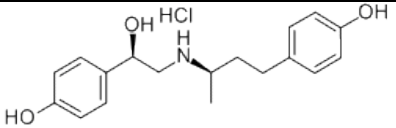
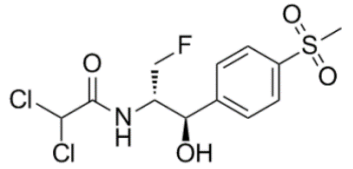
Table S1. The chemical structures of PPCPs molecules and their physicochemical properties.

Compound	Log K_{ow}	pKa	Water solubility (mg/L)	MW g/mol	Chemical Formula	CAS	Structure
Sulfonamides							
Sulfadimethoxine	1.63	5.94	46.3	310.33	C12H14N4O4S	122-11-2	
Sulfamethoxazole	0.89	5.6	610	253.28	C10H11N3O3S	723-46-6	
Sulfamonomethoxine		5.94	10	280.3	C11H12N4O3S	1220-83-3	
Sulfamerazine	0.14	2.29	202	264.3	C11H12N4O2S	127-79-7	
Sulfamethazine	0.14	2.65	150	278.33	C12H14N4O2S	57-68-1	
Sulfachinoxalin	1.68	5.65	>45.1	300.34	C14H12N4O2S	59-40-5	
tetracyclines							

Tetracycline	1.30	3.3	231	444.43	C22H24N2O8	60-54-8	
Oxytetracycline	-0.90	3.27	200	460.43	C22H24N2O9	79-57-2	
Chlorotetracycline		3.3	630	478.88	C22H23ClN2O8	57-62-5	
Doxycycline	0.63	3.09	630	444.43	C22H24N2O8	564-25-0	
quinolones							
Enrofloxacin		6.43	53.9	359.39	C19H22FN3O3	93106-60-6	

Ciprofloxacin	0.28	4.04	86	331.34	C17H18FN3O3	85721-33-1	
Beta-agonist							
Clenbuterol hydrochloride			46.5	313.65	C12H19Cl3N2O	21898-19-1	
Salbutamol	0.64	9.07	17950	239.32	C13H21NO3	18559-94-9	
Cimaterol		13.75		219.28	C12H17N3O	54239-37-1	
Ractopamine	2.4	9.97	4100	301.38	C18H23NO3	97825-25-7	
Chloromycetin							
Florfenicol		10.73		358.21	C12H14Cl2FNO4S	73231-34-2	

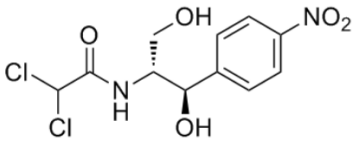
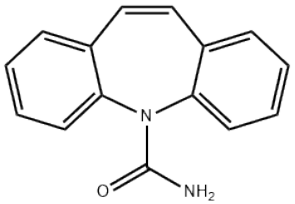
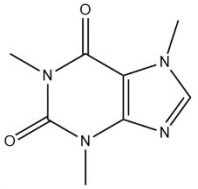
Chloramphenicol	1.14	11.03	2500	323.13	C11H12Cl2N2O5	56-75-7	
anticonvulsan							
Carbamazepine	2.45	13.94	35.4	236.27	C15H12N2O	298-46-4	
Human Indicator							
Caffeine	0.07	10.4	21600	194.194	C8H10N4O2	58-08-2	

Table S2. Optimized MS/MS parameters for PPCPs.

Compound	ESI mode	Precursor ion (m/z)	Product ion (m/z)	Declustering voltage (V)	Entrance voltage (V)	Collision energy (V)	Export voltage (V)
	Positive	311.1	156.1*	130	10	27	9
sulfadimethoxine	Positive	311.1	92.1	130	10	44	16
	Positive	254.1	156.0*	100	10	22	10
sulfamethoxazole	Positive	254.1	92.1	100	10	35	16
	Positive	281.1	108.0	80	10	34	7
sulfamonomethoxine	Positive	281.1	156.0*	80	10	23	13
	Positive	265.1	156.0*	80	10	23	9
sulfamerazine	Positive	265.1	172.1	80	10	22	6
	Positive	279.0	156.0*	90	10	25	5
sulfamethazine	Positive	279.0	186.0	90	10	23	7
	Positive	301.1	156.0*	80	10	21	9
sulfachinoxalin	Positive	301.1	92.1	80	10	38	6
	Positive	445.2	410.1*	160	10	27	17
tetracycline	Positive	445.2	154.1	160	10	35	10
	Positive	462.3	426.0*	100	10	26	18
oxytetracycline	Positive	462.3	443.1	100	10	21	8
	Positive	479.2	462.0	36	10	23	18
chlorotetracycline	Positive	479.2	444.1*	36	10	29	18
	Positive	445.2	428.1*	160	10	24	17
doxycycline	Positive	445.2	154.1	160	10	39	13
	Positive	360.2	342.2*	170	10	29	14
enrofloxacin	Positive	360.2	316.2	170	10	27	5
	Positive	332.1	314.1*	100	10	28	13
ciprofloxacin	Positive	332.1	288.2	100	10	24	6
	Positive	277.1	259.1	60	10	15	7
clenbuterol	Positive	277.1	203.0*	60	10	24	7
	Positive	240.2	166.1	60	10	18	10
salbutamol	Positive	240.2	148.1*	60	10	20	10
	Positive	220.2	116.1	60	10	46	15
cimaterol	Positive	220.2	143.1*	60	10	32	15
	Positive	302.1	284.1*	40	10	16	5
ractopamine	Positive	302.1	164.1	40	10	23	7
	Positive	237.1	194.1*	130	10	26	7
carbamazepine	Positive	237.1	179.1	130	10	46	12
	Positive	195.1	138.1*	90	10	26	8
caffeine	Positive	195.1	110.0	90	10	29	8
	Positive	216.1	174.1*	120	10	23	9
atrazine	Positive	216.1	96.1	120	10	31	7
	negative	320.9	256.8	-110	-10	-15	-10
chloramphenicol	negative	320.9	152.0*	-110	-10	-22	-10
	negative	356.0	185.0	-90	-13	-26	-9
florfenicol	negative	356.0	335.9*	-90	-13	-13	-20

*—represent Quantitative ion.

Table S3. Limits of detection (LOD) of the analytes, linear equation and linearity of calibration.

Compounds	Linear equation (y=ax+b)	R	LOD (ng/L)
sulfadimethoxine	Y=0.18X+0.0743	0.9994	0.25
sulfamethoxazole	Y=0.0749X-0.00716	0.9999	0.25
sulfamonomethoxine	Y=0.0628X-0.00101	0.9999	0.25
sulfamerazine	Y=0.0853X-0.01	0.9999	0.25
sulfamethazine	Y=0.134X+0.168	0.9995	0.25
sulfachinoxalin	Y=0.112X+0.00966	0.9997	0.25
tetracycline	Y=0.0156X-0.0924	0.9906	5
oxytetracycline	Y=0.00813X-0.0696	0.9910	5
chlorotetracycline	Y=0.0105X-0.112	0.9922	5
doxycycline	Y=0.0322X-0.445	0.9935	5
enrofloxacin	Y=0.274X-0.891	0.9984	1
ciprofloxacin	Y=0.125X-2.97	0.9911	1
clenbuterol	Y=0.412X+1.03	0.9951	0.05
salbutamol	Y=0.145X+0.331	0.9949	0.05
cimaterol	Y=0.0871X+0.0836	0.9991	0.05
ractopamine	Y=0.256X+1.42	0.9951	0.05
carbamazepine	Y=0.512X+1.32	0.9949	0.05
caffeine	Y=0.0514X+0.0292	0.9979	2.5
atrazine	Y=0.341X+0.775	0.9978	0.05
chloramphenicol	Y=10700X+18600	0.9995	0.05
florfenicol	Y=15000X+23400	0.9994	0.05

Table S4. The concentration of PPCPs in all sampling points in wet and dry season.

Sampling points	SMX		SMM		SMZ		EFX		CFX		CBZ		CAF		CMP		FFC	
	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry	Wet	Dry
R1	ND	ND	ND	8.60	ND	ND	ND	ND	ND	ND	1.66	ND	815.00	20.30	ND	ND	11.00	1.33
R2	3.40	0.70	0.53	0.67	ND	ND	ND	ND	ND	ND	0.80	ND	85.00	105.50	ND	ND	29.70	2.85
R3	1.63	0.79	0.89	0.79	ND	ND	ND	ND	ND	ND	1.00	ND	77.00	115.50	ND	ND	51.50	4.38
R4	2.41	0.61	0.53	0.83	ND	ND	ND	ND	ND	ND	0.50	ND	135.00	66.50	ND	ND	59.00	2.40
R5	0.90	0.58	1.22	0.69	0.60	0.32	ND	ND	ND	ND	0.15	ND	25.80	74.00	ND	ND	37.05	16.90
R6	10.10	5.90	2.74	0.80	1.01	0.30	ND	ND	ND	ND	0.20	ND	131.00	46.05	ND	ND	56.00	18.65
R7	ND	4.72	1.66	1.07	ND	0.43	ND	ND	ND	ND	0.81	ND	77.00	47.70	ND	ND	12.45	14.85
R8	0.90	ND	ND	13.80	ND	ND	ND	ND	775.00	ND	18.90	ND	127.50	31.35	3.43	ND	14.80	13.05
R9	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.79	ND	114.00	83.50	0.40	ND	26.85	ND
R10	0.50	0.27	ND	0.45	ND	ND	ND	ND	ND	ND	0.15	ND	18.70	65.00	ND	ND	0.15	11.55
R11	3.56	0.25	0.60	ND	ND	0.33	ND	ND	ND	ND	0.30	ND	78.00	57.50	ND	ND	28.00	1.49
R12	ND	0.30	ND	0.28	ND	ND	ND	ND	ND	ND	ND	ND	119.50	32.10	ND	ND	ND	6.25
R13	1.15	0.34	0.55	ND	ND	ND	ND	ND	ND	ND	0.20	ND	53.50	13.95	ND	ND	0.48	ND
R14	2.74	ND	0.79	0.31	2.54	ND	3.74	ND	8.80	ND	0.75	ND	49.65	35.95	0.40	ND	690.00	0.81
R15	ND	14.90	1.33	0.56	0.38	0.55	ND	ND	ND	ND	0.40	ND	34.95	49.40	ND	ND	2.01	4.99
R16	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.30	ND	47.60	4.73	ND	ND	4.42	1.34
R17	1.21	47.15	7.75	3.58	3.24	0.58	ND	ND	ND	ND	ND	ND	23.20	16.85	ND	ND	172.50	12.95
R18	1.05	0.69	2.68	ND	10.50	0.48	2.15	ND	ND	ND	0.35	ND	81.00	36.65	1.34	ND	101.50	24.65
R19	35.25	28.00	1.96	1.98	1.12	0.57	ND	ND	ND	ND	0.51	ND	122.00	81.00	ND	ND	140.50	74.50

ND—not detectable.

Table S5. The EC_{50}, LC_{50} and PNEC of PPCPs to aquatic organism.

Compound	Species	PNEC (ng/L)	MECwet (ng/L)	MECdry (ng/L)	RQwet	RQdry
SMX	Fish	410762	35.25	47.15	8.58E-05	1.15E-04
	Daphnia	1872	35.25	47.15	1.88E-02	2.52E-02
	Green algae	6615	35.25	47.15	5.33E-03	7.13E-03
SMM	Fish	2351876	7.75	13.8	3.30E-06	5.87E-06
	Daphnia	1198	7.75	13.8	6.47E-03	1.15E-02
	Green algae	8772	7.75	13.8	8.83E-04	1.57E-03
SMZ	Fish	291394	10.5	0.58	3.60E-05	1.99E-06
	Daphnia	2045	10.5	0.58	5.13E-03	2.83E-04
	Green algae	6259	10.5	0.58	1.68E-03	9.27E-05
EFX	Fish	4922627	3.74	ND	7.60E-07	0
	Daphnia	504571	3.74	ND	7.41E-06	0
	Green algae	561233	3.74	ND	6.66E-06	0
CFX	Fish	13131424	775	ND	5.90E-05	0
	Daphnia	1240427	775	ND	6.25E-04	0
	Green algae	1621628	775	ND	4.78E-04	0
CBZ	Fish	41330	18.9	ND	4.57E-04	0
	Daphnia	14902	18.9	ND	1.27E-03	0
	Green algae	256	18.9	ND	7.38E-02	0
CAF	Fish	111495	815	115.5	7.31E-03	1.04E-03
	Daphnia	11925	815	115.5	6.83E-02	9.69E-03
	Green algae	772	815	115.5	1.06E+00	1.50E-01
CMP	Fish	883291	3.43	ND	3.88E-06	0
	Daphnia	643462	3.43	ND	5.33E-06	0
	Green algae	185308	3.43	ND	1.85E-05	0
FFC	Fish	6764040	690	74.5	1.02E-04	1.10E-05
	Daphnia	4570401	690	74.5	1.51E-04	1.63E-05
	Green algae	912554	690	74.5	7.56E-04	8.16E-05

MEC—the Max Environmental Concentration; RQ—the Risk quotients corresponding to the maximum environmental concentration.