

**Pharmaceuticals and Personal Care Products across Different Water Bodies in Taihu Lake
Basin, China: Occurrence, Source, and Flux**

Supplemental Material:

Content:	
SM-1	Figure S1. Schematic diagrams of the treatment processes in the two WWTPs.
SM-2	Figure S2. PPCP concentrations in the different land use types in four seasons.
SM-3	Table S1. Physicochemical property and molecular of target PPCPs.
SM-4	Table S2. Each sampling site with corresponding river and sub-region of Taihu Lake.
SM-5	Table S3. Parameter settings of solid phase extraction.
SM-6	Table S4. Mobile phase elution procedures.
SM-7	Table S5. Mass spectrometry conditions for 13 PPCPs.
SM-8	Table S6. The mean removal rates of PPCPs in three processes used by two WWTPs.

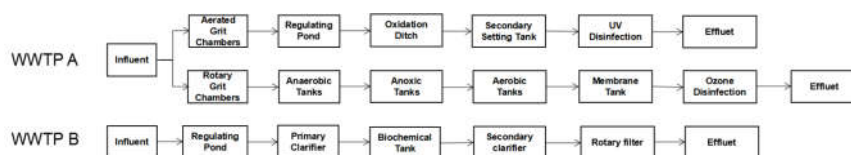


Figure S1. Schematic diagrams of the treatment processes in the two WWTPs.

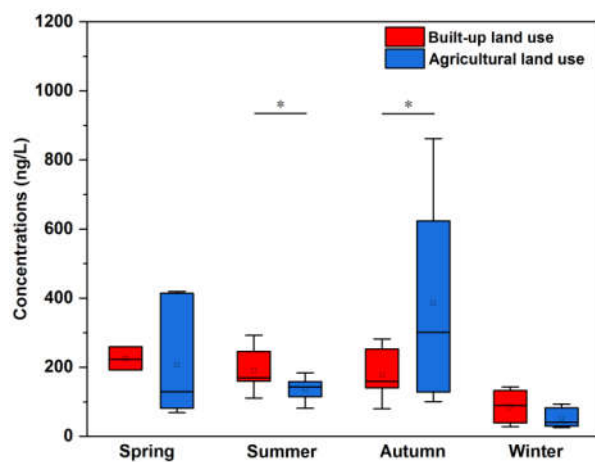


Figure S2. PPCP concentrations in different land use types in four seasons. The symbols “*” indicate statistically significant difference at 0.05 level (two-tailed).

Table S1. Physicochemical property and molecular of target PPCPs.

Compound	Abbreviation	CAS Number	Molecular Formula	Relative Molecular Mass	log K_{ow}
roxithromycin	ROX	80214-83-1	C ₄₁ H ₇₆ N ₂ O ₁₅	837.05	3.1
clarithromycin	CLR	81103-11-9	C ₃₈ H ₆₉ NO ₁₃	747.95	3.2
fluoxetine	FLX	54910-89-3	C ₁₇ H ₁₈ F ₃ NO	309.33	4.0
citalopram	CTP	219861-08-2	C ₂₀ H ₂₁ FN ₂ O	324.39	3.2
sertraline	SER	79617-96-2	C ₁₇ H ₁₇ Cl ₂ N	306.23	4.8
metoprolol	MTL	37350-58-6	C ₁₅ H ₂₅ NO ₃	267.36	1.9
bezafibrate	BZB	41859-67-0	C ₁₉ H ₂₀ ClNO ₄	361.82	3.8

gemfibrozil	GFB	25812-30-0	C ₁₅ H ₂₂ O ₃	250.33	3.8
n, n-diethyl-m-toluamide	DEET	134-62-3	C ₁₂ H ₁₇ NO	191.27	2.0
triclocarban	TCC	101-20-2	C ₁₃ H ₉ Cl ₃ N ₂ O	315.58	5.3
clotrimazole	CTM	23593-75-1	C ₂₂ H ₁₇ ClN ₂	344.84	5.0
caffeine	CFI	58-08-2	C ₈ H ₁₀ N ₄ O ₂	194.19	-0.1
carbamazepine	CBZ	298-46-4	C ₁₅ H ₁₂ N ₂ O	236.27	2.5

Table S2. Each sampling site with corresponding river and sub-region of Taihu Lake.

Environmental Compartments	Sampling Sites	Location
WWTPs	WWTP A	120.3343°E,31.6107°N
	WWTP B	120.8467°E,31.6123°N
Rivers	R1	120.8296°E,31.7805°N
	R2	120.7985°E,31.7611°N
	R3	120.6433°E,31.6518°N
	R4	120.5998°E,31.5379°N
	R5	120.5709°E,31.5044°N
	R6	120.4193°E,31.4515°N
	R7	120.8985°E,31.7806°N
	R8	120.7622°E,31.5992°N
	R9	120.5057°E,31.3343°N
	R10	120.8223°E,31.6938°N
	R11	120.3573°E,31.4734°N
	R12	120.1278°E,31.5071°N
	R13	120.0371°E,31.4989°N
	R14	120.0102°E,31.4604°N

Taihu Lake	R15	120.0106°E,31.4281°N
	R16	119.9536°E,31.3603°N
	R17	119.9315°E,31.3212°N
	L1	120.0472°E,31.4258°N
	L2	120.1728°E,31.4686°N
	L3	120.1622°E,31.3966°N
	L4	120.2462°E,31.3789°N
	L5	120.3757°E,31.4478°N
	L6	120.2453°E,31.5156°N
	L7	120.2292°E 31.3103°N
	L8	120.2697°E 31.2328°N
	L9	120.4590°E 31.1717°N
	L10	119.9639°E 31.3111°N
	L11	119.9583°E 31.2167°N
	L12	120.0119°E 31.1364°N
	L13	120.1347°E 30.9931°N
	L14	120.0257°E 31.0664°N
	L15	120.2996°E 31.0017°N
	L16	120.0969°E 31.3333°N
	L17	120.1033°E 31.2258°N
	L18	120.1505°E 31.0628°N
	L19	120.2676°E 31.0136°N
	L20	120.1897°E 31.1347°N

Table S3. Parameter settings of solid phase extraction.

Operation	Solvent	Flow (mL/min)	volume (mL)
Condition	methanol	5	5
	ultrapure water	5	5
Sample loading	sample	10	1000
Elute	methanol	5	5
	Methanol:acetone (v/v 1:1)	5	5

Table S4. Mobile phase elution procedures.

Gradient (min)	Flow (mL/min)	Mobile Phase A %	Mobile Phase B %
0	0.4	90	10
0.25	0.4	90	10
3.00	0.4	5	95
4.00	0.4	5	95
4.01	0.4	90	10
5	0.4	90	10

Mobile phase A: 0.1% formic acid; Mobile phase B: 100% acetonitrile.

Table S5. Mass spectrometry conditions for 13 PPCPs.

Compound	Retention Time (ms)	Precursor Ion (m/z)	Product Ions (m/z)	Cone Voltage (V)	Collision Energy (eV)	Modes
ROX	7	837.50	158.0	37	30	ESI+
CLR	7	748.40	158.20	40	30	ESI+
FLX	7	310.13	43.99	6	10	ESI+
			147.99		8	
CTP	8	325.10	108.93	38	26	ESI+
			262.03		20	
SER	11	306.10	158.86	20	26	ESI+
			274.97		12	
MTL	36	268.2	116.0	30	18	ESI+
			133.0		24	
BZB	27	360.27	153.90	26	26	ESI-
			274.03		16	
GFB	70	251.03	82.95	18	12	ESI+
			128.93		10	
DEET	27	192.13	90.93	38	28	ESI+
			118.95		18	
TCC	70	314.97	161.85	28	16	ESI-
			162.17		26	
CTM	17	277.07	160.94	42	20	ESI+
			164.98		22	
CFI	45	195.07	110.03	40	24	ESI+
			138.04		22	
CBZ	7	236.97	165.0	30	42	ESI+
			178.87		34	

Table S6. The mean removal rates of PPCPs in three processes used by two WWTPs.

Compound	Removal Rates (%) in WWTP A		Removal Rates (%) in WWTP B
	OD Process	MBR Process	A ² O Process
ROX	−289.4	−29.1	−892.4
CLR	/	/	−1593.8
MTL	−66.2	57.6	77.9
BZB	100.0	100.0	−142.9
GFB	/	/	56.7
DEET	82.6	82.2	−320.8
CFI	98.6	97.6	77.6
CBZ	−104.6	−38.8	−244.5