

Effect of background water matrices on pharmaceutical and personal care products removal by UV-LED/TiO₂

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Data analysis

Equation S1: Removal% during dark period

$$\text{Removal \%} = \frac{C_0 - C_f}{C_0} \times 100 \quad (1)$$

C_0 is the initial concentration (Table S1) and C_{60} in the concentrations at t=60 min.

Equation S2: Langmuir-Hinshelwood kinetics model

$$\ln \frac{C_t}{C_0} = -k_{app}t \quad (2)$$

C_0 and C_t are the concentrations at t=0 min and throughout the exposure period, respectively and k_{app} is the apparent first order reaction rate constant (min^{-1})

Equation S3: EEO

$$EEO = \frac{1000 Pt}{V \log(\frac{c_i}{c_f})} \quad (4)$$

P is the rated power (kW), V is the volume of treated water (L) in the time t (h), and c_i and c_f are the initials and final concentrations, respectively.

Table S1. Studies in photocatalytic degradation of pharmaceuticals and personal care compounds in different water matrices

No.	Water Matrix	PPCP	Photocatalyst	light condition	Ref.
1	Ultrapure water	DCF, CBZ, SMX	Activated Carbon doped with TiO ₂	Xenon lamp (300 W)	[1]
2		DCF	TiO ₂	UV-C, solar irradiation	[2]
3		MER	TiO ₂ immobilized on fiber glass	UV lamps (8 W)	[3]
4		ANT	TiO ₂ - Reduced graphene oxide	UV-A (38 W m ⁻²), Visible irradiation (307 38 W m ⁻²)	[4]
5		ACE, IBU, ANT	Activated Carbon doped with TiO ₂	Xenon lamp (765 W m ⁻²)	[5]
6		TC	TiO ₂	UV-B lamp (7 W)	[6]
7		ATEN, ATOR, o-ATOR, p-ATOR, ATRZ, CBZ, eCBZ, DCF, FLX, NFLX, GFZ, IBU, NPX, SULF, TCS, TCB, TRIM, VEN	porous titanium – titanium dioxide (PTT) substrates	Controlled periodic illumination UV-LED (1.7×10 ⁻³ W)	[7]
8		DCF	Sulfur doped TiO ₂	Visible light	[8]
9		4-CP, NPX	Nickel, iron and copper doped with TiO ₂	UV lamps (15 W)	[9]
10		IBP, CTZ, NPX	TiO ₂ immobilized on polyacrylonitrile/multiwall carbon nanotubes	Visible light (125 W), Xenon lamp	[10]
11		CBZ	TiO ₂ / Ti ₃ C ₂ T _x	UV light, Solar light	[11]
12		ACE	TiO ₂ - Tungsten trioxide	Xenon lamp (500 W)	[12]
13		β blocker	Platinum doped with TiO ₂ - Reduced graphene oxide-	Xenon lamp (300 W)	[13]
14		Phenol	Epoxy TiO ₂ sand composite	UV-A lamps (15 W)	[14]
15		ACE	TiO ₂ - pristine carbon nanotubes	High-pressure mercury lamp (7.53 mW m ⁻²)	[15]
16		BPA	Nickel doped with TiO ₂	Visible light (25 W)	[16]
17		4-CP	Nitrogen doped with TiO ₂	Visible LED (100 W)	[17]

18	CBZ, SMZ, IBP	TiO ₂ - Reduced graphene oxide immobilized on optical fiber	High-pressure UV Mercury vapor lamp (160 W)	[18]
19	DCP, BPA, IBU, FLU	Boron doped with TiO ₂	Visible light irradiation (150 W)	[19]
20	ATEN, ATOR, ATZ, CBZ, DCF, FLX, GEM, IBU, MON, NPX, SULF, TCS, TCB, TRIM, VEN	TiO ₂	UV-LED (1.7×10^{-3} W)	[20]
21	CBZ, SMZ, IBP	TiO ₂ - Reduced graphene oxide, Iron doped TiO ₂	Visible light source (150W)	[21]
22	ATEN, ATOR, o-ATOR, p-ATOR, ATRZ, CBZ, DCF, FLX, NFLX, GFZ, IBU, NPX, SULF, TCS, TCB, TRIM, VEN	TiO ₂ immobilized onto quartz fiber filters and porous titanium sheets	UV-LED (1.7×10^{-3} W)	[22]
23	DMX	Silver doped TiO ₂	UV-C (20 W)	[23]
24	IBU	Bismuth and nickel doped with TiO ₂	UV (36 W)	[24]
25	MBC, DMI	Iron doped with TiO ₂	Solar light (600 W m^{-2}), UV light (30 W m^{-2})	[25]
26	ACT, DCF, IBP, SMX,	TiO ₂	UV-C, UV-B, UV-A (10 mW)	[26]
27	ACV	TiO ₂ - graphitic carbon nitride	Visible light (30 mW m^{-2})	[27]
28	EZ	Platinum doped TiO ₂ film	UV (10 W)	[28]
29	DCF, ACE, AMX, AMP	Activated carbon doped TiO ₂	Solar UV (30 W m^{-2})	[29]
30	CIP	TiO ₂	UV-C	[30]
31	BPA, CBZ	Multiwall carbon nanotubes- TiO ₂ - SiO ₂	UV light (1 mW m^{-2})	[31]
32	SP	Nitrogen doped TiO ₂	UV-LED light (32 mW m^{-2})	[32]
33	IFO, CP, TRO	TiO ₂	UV-A (8 W)	[33]
34	IBP, CBZ, ATEN	Immobilized TiO ₂ with calcium alginate beads	UV-A light (38 mW m^{-2}), Visible light (307 mW m^{-2})	[34]
35	ACP	Nitrogen doped TiO ₂	Visible light	[35]
36	TCA	carbon doped TiO ₂	Visible light	[36]

37	NB, MTZ	Silver doped hollow TiO ₂	High pressure mercury lamp (125 W)	[37]	
38	4-NP	Iron doped with TiO ₂	Visible light (150 W)	[38]	
39	MMA	Nitrogen doped TiO ₂	Natural sun light, UV light	[39]	
40	AMX, 2,4-DCP	Silver doped TiO ₂	Visible light (180 W m ⁻²)	[40]	
41	OFX	Nickel doped TiO ₂	Solar light	[41]	
42	CHD	TiO ₂	UV-A (10 W)	[42]	
43	ACE, SMZ, CMT, PRO	TiO ₂ nanofibers	UV-A (10 W)	[43]	
44	LEVO	TiO ₂	UV-C	[44]	
45	CAP	Silver doped TiO ₂	UV (30W)	[45]	
46	AMX	Lead doped TiO ₂	UV-C (15 W)	[46]	
47	2,4-DCP	Chromium doped TiO ₂	Visible light halogen lamp (1000 W)	[47]	
48	VEN, FLX, SMZ	TiO ₂ nano wire	Pressure mercury lamp (2.7×10^{-4} W m ⁻²)	[48]	
49	NFLX, ATOR, TRIM, ATRZ, LIN, FLX, VEN, SMZ, DCF, TRIM, BPA, GEM, ATRZ, CBZ, IBU	TiO ₂ nano wire	Pressure mercury lamp (2.7×10^{-4} W m ⁻²)	[49]	
50	IBP, ATEN, CBZ	Alginate supported TiO ₂	UV light (80×10^{-6} W m ⁻²)	[34]	
51	INH, Sulfa, Trim, NFIX, Lin, MXF, MTZ	TiO ₂ - Biobased polyethylene terephthalate	Xenon lamp (1.5 kW)	[44]	
52	BPA	Zirconium doped TiO ₂	UV light (20 W)	[50]	
53	SCP, SPR, SMZ	TiO ₂	High-pressure mercury lamp (125 W)	[51]	
54	Surface water	DCF, MEM	TiO ₂ -SnS ₂ nanocomposite	Xenon arc lamp (450 W)	[52]
55	CIP, OFX	TiO ₂	Solar light (1366 W m ⁻²)	[53]	
56	SMZ	TiO ₂	UV-C (0.5 mW m ⁻²)	[54]	
57	CBZ, SMZ	Magnetic carbon nanotube-TiO ₂ Composites	Solar simulator (1000 W m ⁻²)	[55]	

58	CBZ, GEM, TRIM, WAR, MET	TiO ₂ film deposited on a stainless-steel mesh	Mercury low pressure UV lamp (40 W)	[56]	
59	BPA	Nitrogen, fluorine co-doped TiO ₂	Simulated sunlight xenon lamp (1600 W)	[57]	
60	CBZ	Nitrogen doped TiO ₂	Solar simulator xenon arc lamp (150 W)	[58]	
61	ACE, ATEN, ATOR, o-ATOR, p-ATOR, ATRZ, CAFF, CBZ, eCBZ, DESVEN, DCF, FLX, NFLX, GEM, IBU, NPX, MON, SMZ, SULF, TCS, TRIM, VEN	Silver doped TiO ₂	UV-LED (2060 and 2300 mW)	[59]	
62	Wastewater effluent	GEM, NPX, HCT	TiO ₂	UV-A (10 W)	[60]
63	CBZ, DCF, TRIM	Nitrogen doped TiO ₂ , Iron doped TiO ₂	Direct sunlight ($29.7 \pm 5.3 \text{ W m}^{-2}$)	[61]	
64	ACT, FRS, NMD, DZP	TiO ₂	UV-A, UV-C (6 W)	[62]	
65	CBZ, DCF, IOP, GEM, MET, SMZ, TRIM, WAR	Immobilized TiO ₂ on PVDF dual layer hollow fiber membrane	UV lamps (40 W)	[63]	
66	IBU	TiO ₂	UV high intensity LEDs (10 W)	[64]	
67	DCF, CAFF, IFO, FP, RXM, AZM	TiO ₂	Sunlight exposure	[65]	
68	MTZ	Iron doped TiO ₂	UV-C (125 W)	[66]	
69	TCS	Carbon nanotube doped TiO ₂	UV-C (6 W)	[67]	
70	ACE, ANT, CAFF, KET, MET, SMZ, CBZ, HCT, DCF	TiO ₂	Solar irradiation	[68]	
71	DCF, CBZ, IBU, PRO	TiO ₂ immobilized on quartz sand	simulate solar light, Xenon high (55 W)	[69]	
72	CMT, PRO, CBZ	Immobilized electrospun TiO ₂ nanofiber	UV (4 W)	[70]	
73	ATEN, HCT, OFX, TRIM	TiO ₂	UV (30 W m^{-2})	[71]	
74	MTN, CLT, BFN, CBZ, DCF, SMX	TiO ₂	Xenon lamp (1500 W)	[72]	

75	FLX, DCF, CBZ, BPA, OFX,NFLX, GEM, PAR, CLOT, AZM, LOR, PRO, FRS, HCT,FN, Losartan, KETO, CR, FCZ, CPFX, Xanax, TRF, TCA,HHCB, MK, AHTN	TiO ₂	UV light	[73]
76	BPA	TiO ₂	UV-A (0.7 W)	[74]
77	USAN, ATEN, ATRZ, AZM, BZF, CAFF, CBZ, CPFX, IBU, INDO, IPU, KETO, LIN, NPX, NIC, NFLX, OFX, PX, PRAV, PRMB, PRO, PP, R, SBL, SIM, SMZ, TRIM, VEN	TiO ₂	Solar simulator xenon lamp (765 W m ⁻²)	[75]
78	OFX, ACE, DCF, CAF, CBZ, TRIM, TBZ, ACP	TiO ₂	UV, xenon lamp (300 W)	[76]
79	CBZ	Membrane bioreactor TiO ₂	UV-A (8 W)	[77]
80	ATEN, PRO	TiO ₂	Solar simulator xenon lamp (1000 W)	[78]

Table S2. Pharmaceuticals and personal care products (PPCP) and their abbreviations

PPCP	Abb.	PPCP	Abb.
Acephate	APT	Isoniazid	INH
Acetaminophen	ACE	Isoproturon	IPU
Acetamiprid	ACP	Iopromide	IOP
Acyclovir	ACV	Ketoprofen	KeTO
Alprazolam	Xanax	Ketorolac	KET
Amoxicillin	AMX	Levofloxacin	LEVO
Ampicillin	AMP	Lincomycin	LIN
Antipyrine	ANT	Lorazepam	LOR
Atenolol	ATEN	Malathion	MMA
Atorvastatin	ATOR	Memantine	MEM
o-Hydroxy atorvastatin	o-ATOR	Meropenem	MER
p-Hydroxy atorvastatin	p-ATOR	mesotrione	MTN
Atrazine	ARTZ	Metoprolol	MET
Azithromycin	AZM	Metronidazole	MTZ
bifenthrin	BNF	Monensin	MON
Benzafibrate	BZF	Moxifloxacin	MXF
Bisphenol A	BPA	Musk ketone	MK
Caffeine	CAFF	4-nitrophenol	4-NP
Carbamazepine	CBZ	Naproxen	NPX
Carvedilol	CR	Nicotine	NIC
10,11-Epoxyde Carbamazepine	eCBZ	Nimesulide	NMD
Cetirizine	CTZ	Nitrobenzene	NB
Chloramphenicol	CAP	Nimesulide	NMD
4-chlorophenol	4-CP	Norfluoxetine	NFLX
Chlorhexidine Digluconate	CHD	Ofloxacin	OFX
Cimetidine	CMT	Pravastatin	PRAV
Ciprofloxacin	CIP	Paraxanthine	PX
Clothianidin	CLT	Paroxetine	PAR
Clotrimazole	CLOT	Primidone	PRMB
Cyclophosphamide	CP	Propyphen.	PP
Desvenlafaxine	DESVEN	Propranolol	PRO
Dexamethasone	DXM	Spiramycin	SP
Diazepam	DZP	Sulfachlorpyridazine	SCP
Diclofenac	DCF	Sulfamethazine	SMZ
2,4-dichlorophenol	2,4-DCP	Sulfamethoxazole	SULFA
Ethenzamide	EZ	Sulfapyridine	SPR

Fenofibrate	FN	Ranitidine	R
Fenoprofen	FP	Roxithromycin	RXM
Flurbiprofen	FLU	Salbutamol	SBL
Fluconazole	FCZ	Simazine	SIM
Fluoroquinolone	FQ	Tetracycline	TC
Fluoxetine	FLX	Terbinafine	TRF
Furosemide	FRS	thiabendazole	TBZ
Galaxolide	HHCB	Tonalide	AHTN
Gemfibrozil	GEM	2,4,6-Trichloroanisole	TCA
Hydrochlorothiazide	HCT	Triclosan	TCS
Ibuprofen	IBU	Trimethoprim	TRIM
Ifosfamide	IFO	Trofosfamide	TRO
Indomethacine	INDO	Venlafaxine	VEN
		Warfarin	WAR

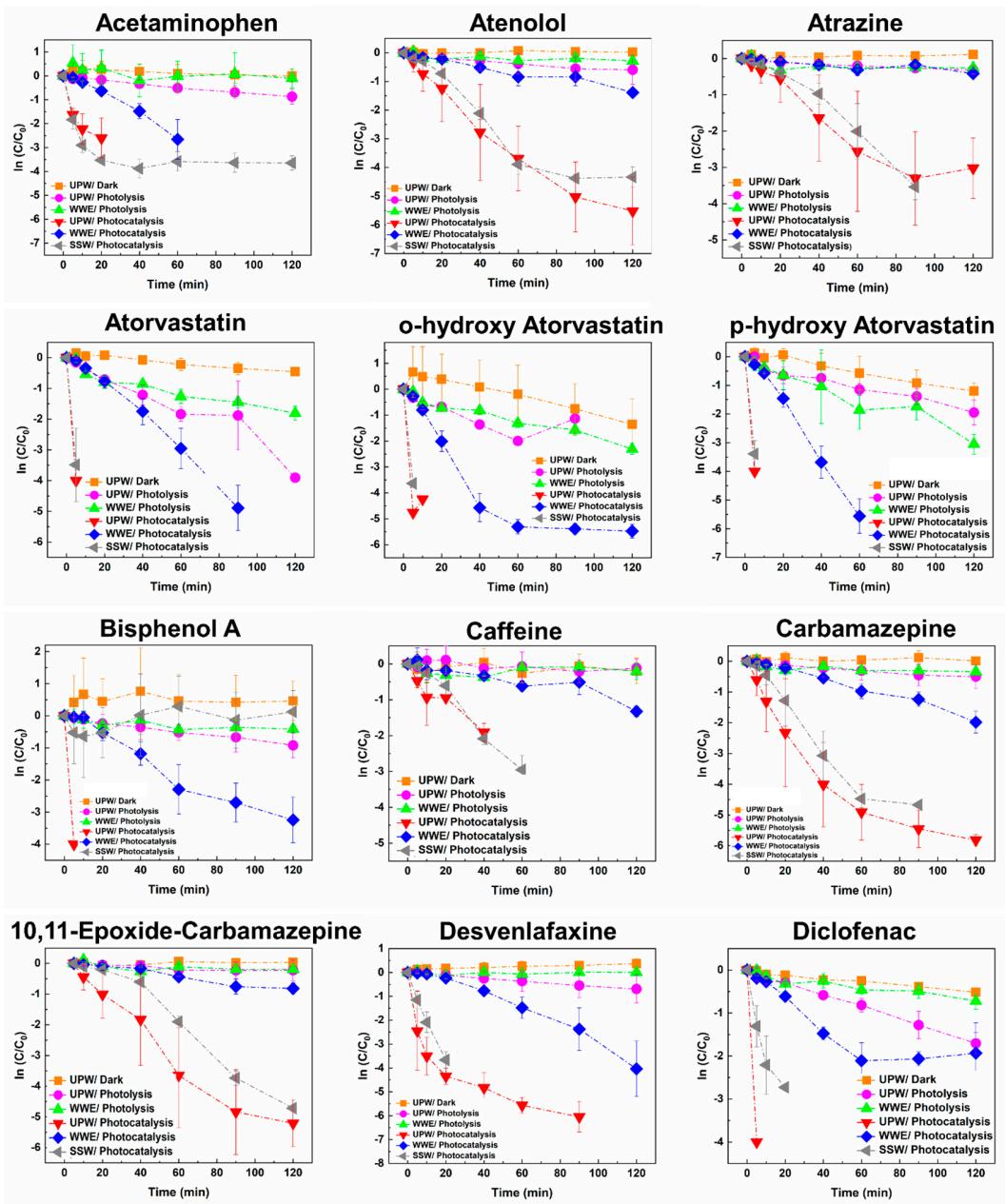


Fig. S1 (continued) Removal of targeted PPCPs in ultrapure water (UPW), wastewater effluent (WWE), and synthetic surface water (SSW) under dark (120 min dark irradiation using P25), photolysis (120 min under UV-LED irradiation without P25) and photocatalysis (120 min under UV-LED irradiation and using P25) treatments.

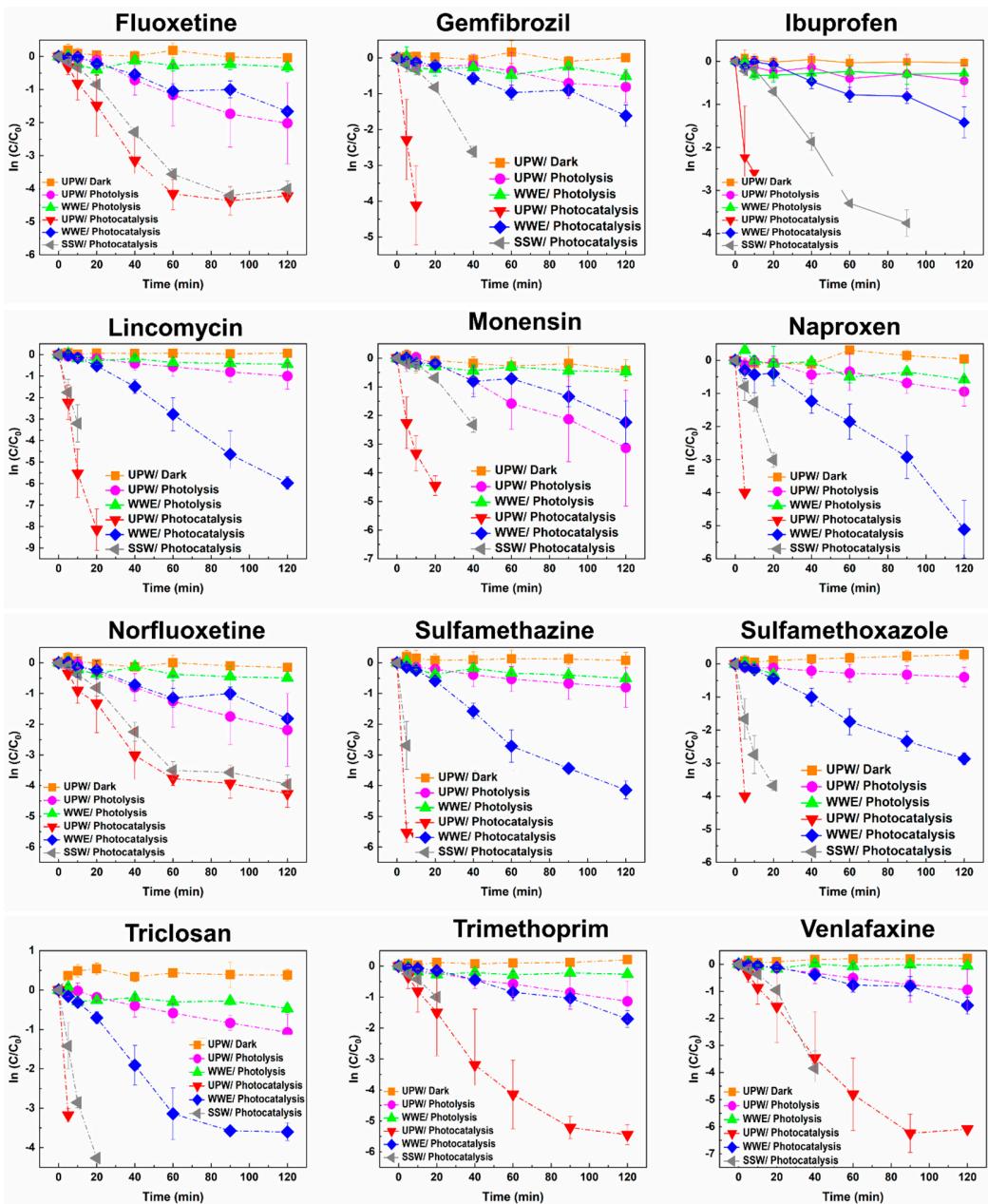


Fig. S1 (continued) Removal of targeted PPCPs in ultrapure water (UPW), wastewater effluent (WWE), and synthetic surface water (SSW) under dark (120 min dark irradiation using P25), photolysis (120 min under UV-LED irradiation without P25) and photocatalysis (120 min under UV-LED irradiation and using P25) treatments.

Table S3. *p*-values for One-Way ANOVA tests (SigmaPlot, $\alpha=0.05$) during 60 min equilibrium period, photolysis and photocatalysis. Tukey tests (multiple comparisons) were conducted when a statistical significance was detected with overall statistical significance level of 0.05.

Compound	Equilibrium Period			Photolysis	Photocatalysis		
	UPW vs. SSW	UPW vs. WWE	SSW vs. WWE		MQW vs. SSW	MQW vs. WWE	SSW vs. WWE
Acetaminophen	No	No	No	No	No	Yes	Yes
<i>p</i> -value	0.223	0.223	0.223	0.124	0.206	0.002	<0.001
Atenolol	No	No	No	No	No	Yes	No
<i>p</i> -value	0.450	0.450	0.450	0.432	0.631	0.022	0.056
Atorvastatin	No	No	No	Yes	No	Yes	Yes
<i>p</i> -value	0.283	0.283	0.283	0.002	0.0305	0.003	0.012
o-Hydroxy Atorvastatin	Yes	Yes	No	Yes	No	Yes	Yes
<i>p</i> -value	0.02	0.002	0.176	0.167	0.593	0.013	0.003
p-Hydroxy Atorvastatin	No	Yes	No	Yes	No	Yes	Yes
<i>p</i> -value	0.056	0.018	0.056	0.005	0.560	0.007	0.017
Atrazine	No	No	No	No	No	Yes	No
<i>p</i> -value	0.790	0.790	0.790	0.290	0.823	0.037	0.062
Bisphenol A	Yes	Yes	No	No	Yes	Yes	Yes
<i>p</i> -value	0.004	0.003	0.995	1	<0.001	<0.001	0.022
Caffeine	No	No	No	Yes	No	No	No
<i>p</i> -value	0.486	0.486	0.486	0.048	0.145	0.145	0.145

Carbamazepine	No	No	No	No	No	No	No
<i>p-value</i>	0.436	0.436	0.436	0.783	0.069	0.069	0.069
10,11-Epoxide Carbamazepine	No	No	No	No	No	Yes	No
<i>p-value</i>	0.927	0.927	0.927	0.602	0.165	0.014	0.150
Desvenlafaxine	No	No	No	No	No	Yes	Yes
<i>p-value</i>	0.099	0.099	0.099	0.099	0.154	<0.001	<0.009
Diclofenac	Yes	Yes	No	Yes	Yes	No	Yes
<i>p-value</i>	0.016	0.006	0.649	0.006	0.009	0.971	0.012
Fluoxetine	No	No	No	No	Yes	Yes	Yes
<i>p-value</i>	0.426	0.426	0.426	0.416	0.020	<0.001	0.001
Gemfibrozil	No	No	No	No	Yes	Yes	No
<i>p-value</i>	0.05	0.05	0.05	0.05	<0.001	<0.001	0.685
Ibuprofen	No	No	No	No	Yes	Yes	No
<i>p-value</i>	0.113	0.113	0.113	0.113	0.004	0.011	0.840
Lincomycin	No	No	No	No	No	Yes	Yes
<i>p-value</i>	0.506	0.506	0.506	0.554	0.154	<0.001	0.002
Monensin	Yes	Yes	No	No	Yes	Yes	No
<i>p-value</i>	0.019	0.011	0.790	0.230	0.003	0.002	0.769
Naproxen	No	No	No	No	Yes	Yes	Yes
<i>p-value</i>	0.255	0.255	0.255	0.565	<0.001	<0.001	0.010
Norfluoxetine	No	No	No	No	No	Yes	No

<i>p</i> -value	0.417	0.417	0.417	0.417	0.403	0.03	0.153
Sulfamethazine	No	No	No	Yes	No	Yes	Yes
<i>p</i> -value	0.283	0.283	0.283	0.033	0.163	0.003	0.023
Sulfamethoxazole	No	No	No	No	Yes	Yes	No
<i>p</i> -value	0.712	0.712	0.712	0.122	0.022	0.008	0.548
Triclosan	No	No	No	No	No	yes	No
<i>p</i> -value	0.330	0.330	0.330	0.330	0.159	0.037	0.445
Trimethoprim	No	No	No	No	No	Yes	No
<i>p</i> -value	0.762	0.762	0.762	0.762	0.236	0.027	0.225
Venlafaxine	No	No	No	No	No	Yes	No
<i>p</i> -value	0.578	0.578	0.578	0.578	0.075	0.009	0.204

Table S4. PPCPs types and number of bonds

PPCPs	#rings	aromatic ring	#OH (Hydroxy)	H bond acceptor	H bond donor	Carboxyl (COOH)	Anisole (OCH3)	Methyl (CH3)	Amide (NHCO)
BPA	2	2	2	2	2			2	
NPX	2	2	-	3	1	1	1	1	
ATOR	4	4	3	5	4	1		2	1
pATOR	4	4	3	5	4	1		2	1
oATOR	4	4	3	6	5	1		2	1
SULF	2	2		4	2		1	1	0
TCS	2	2	1	1	1				
SMZ	2	2		5	2			2	0
IBU	1	1		2	1	1		3	
LIN	2	0	4	7	5			4	
GFZ	1	1		3	1	1		4	1
MON	5	0	3	11	4	1		8	
desVEn	2	1	2	3	2			2	
ACE	1	1	2	3	2			1	
CBZ	3	2							
eBCZ	3	4	2	2	1				
VEN	2	1	1	3	1		1	2	
CAFF	2	2		3				3	
TRIM	2	2		7	2		3	3	
NFLX	3	2		6	2	1		1	
ATEN	1	1	1	4	3			2	
FLX	2	2		2	1			1	

ATRZ	1	1		5	2			3	
DCF	2	2		3	2	1			1

, The PCA analysis couldn't provide required scores due to the lack of data points

Table S5. Correlation coefficient in PCA matrix

Variables	UPW	SSW	WWE
Charge	-0.45	-0.33	-0.26
Log D_{ow}	0.53	0.40	0.45
Solubility	-0.53	-0.50	-0.57
Weight	0.34	0.65	0.58

*Correlation matrix calculated using principle component analysis function (multivariate analysis), OriginPro 8.

Table S6. Extracted Eigenvectors in three water matrices

	UPW		SSW		WWE	
	PC1 (60.36%)	PC2 (16%)	PC1 (49.7%)	PC2 (26.7%)	PC1 (58.09%)	PC2 (18.05%)
Charge	-0.41	0.51	-0.14	0.68	-0.37	0.68
Log D_{ow}	0.52	-0.20	0.49	0.40	0.47	-0.14
Solubility	-0.51	-0.15	-0.53	-0.42	-0.51	-0.05
Weight	0.35	0.81	0.46	-0.32	0.37	0.72

Table S7. Total organic carbon for **wastewater effluent** upon collection from the Waterloo treatment plant and after photocatalytic tests were performed on the matrix.

Inorganics	Units	Waterloo Treatment Plant	120 min dark treatment	120 min photolysis	120 min photocatalysis

Total Organic Carbon (TOC)	mg L ⁻¹	9.37	8.70	8.20	6.90
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Table S8. *p*-values for One-Way ANOVA tests (SigmaPlot, $\alpha=0.05$) for EEO. Tukey tests (multiple comparisons) were conducted when a statistical significance was detected with overall statistical significance level of 0.05.

Compound	UPW vs. SSW	UPW vs. WWE	SSW vs. WWE
Acetaminophen	No	Yes	Yes
<i>p</i> -value	0.988	0.023	0.014
Atenolol	No	Yes	Yes
<i>p</i> -value	0.877	<0.001	<0.001
Atorvastatin	Yes	Yes	Yes
<i>p</i> -value	0.002	0.019	<0.001
o-Hydroxy Atorvastatin	No	Yes	Yes
<i>p</i> -value	0.989	<0.001	<0.001
p-Hydroxy Atorvastatin	No	Yes	Yes
<i>p</i> -value	0.809	<0.001	<0.001
Atrazine	No	Yes	Yes
<i>p</i> -value	0.578	<0.001	<0.001
Bisphenol A	Yes	Yes	Yes
<i>p</i> -value	0.025	<0.001	<0.001
Caffeine	No	Yes	Yes
<i>p</i> -value	0.594	<0.001	<0.001
Carbamazepine	No	Yes	Yes
<i>p</i> -value	0.995	<0.001	<0.001

10,11-Epoxide Carbamazepine	No	Yes	Yes
<i>p</i> -value	0.611	<0.001	<0.001
Desvenlafaxine	No	Yes	Yes
<i>p</i> -value	0.343	0.004	<0.001
Diclofenac	No	No	No
<i>p</i> -value	0.967	0.967	0.967
Fluoxetine	No	Yes	Yes
<i>p</i> -value	0.845	<0.001	<0.001
Gemfibrozil	No	Yes	Yes
<i>p</i> -value	0.163	<0.001	<0.001
Ibuprofen	No	Yes	Yes
<i>p</i> -value	0.148	0.001	<0.001
Lincomycin	No	Yes	Yes
<i>p</i> -value	0.393	0.001	<0.001
Monensin	No	Yes	Yes
<i>p</i> -value	0.345	0.007	0.002
Naproxen	Yes	Yes	Yes
<i>p</i> -value	0.026	<0.001	<0.001
Norfluoxetine	No	Yes	Yes
<i>p</i> -value	0.689	<0.001	<0.001
Sulfamethazine	No	Yes	Yes
<i>p</i> -value	0.831	<0.001	<0.001
Sulfamethoxazole	Yes	Yes	Yes
<i>p</i> -value	0.011	<0.001	<0.001
Triclosan	No	Yes	Yes

<i>p</i> -value	0.261	<0.001	<0.001
Trimethoprim	No	Yes	Yes
<i>p</i> -value	1	<0.001	<0.001
Venlafaxine	No	Yes	Yes
<i>p</i> -value	0.903	<0.001	<0.001

Table S9. Chemical and physical properties of targeted PPCPs in three water matrices and their concentrations UPW = ultrapure water; SSW = synthetic surface water; WWE = wastewater effluent

	UPW				SSW				WWE				
	charge ^a	logD ^b	log S ^c	Conc. ^d	Charge	LogD	Log S	Conc.	Charge	LogD	log S	Conc.	MW
ACE	0	0.91	-1.132	1.6	-0.03	0.89	-1.12	1.96	0	0.906	-1.131	0.04	151.16
ATEN	1	-2.678	0.428	2	0.98	-1.24	0.1	1.96	1	-2.14	0.428	0.01	266.34
ATOR	-0.98	3.7	-5.34	1.92	-1	2.09	-3.36	1.72	-1	2.76	-4.36	0.05	558.64
pATOR	0	5.75	-7.37	1.03	-0.04	5.75	-7.37	1.92	0	5.75	-7.37	0.09	556.63
oATOR	-0.98	3.3912	-4.86	1.32	-1.15	1.71	-2.8	1.8	-1.01	2.44	-3.86	0.1	574.65
ATRZ	0	2.19	-3.79	2.18	0	2.2	-3.8	2.08	0	2.19	-3.8	0	214.68
BPA	0	4.04	-3.18	1.69	-0.02	4.04	-3.18	2.85	0	4.04	-3.18	0.03	228.29
CAFF	-0.02	-0.55	-0.44	2.8	-0.68	-0.55	-0.44	2.44	-0.17	-0.55	-0.44	0.01	194.19
CBZ	0	2.77	-3.79	2.52	0	2.77	-3.79	2.4	0	2.77	-3.79	0.02	236.27
eBCZ	0.08	1.97	-3.33	2.69	0	1.97	-3.33	2.52	0.01	1.97	-3.33	0.01	236.27
desVEN	1	-0.22	0	1.08	0.87	1.63	-1.24	1.64	0.98	0.687	-0.286	0.03	263.37
DCF	-0.99	2.263	-2.289	1.69	-1	0.855	-0.29	3.04	-1	1.368	-1.293	0.03	296.15
FLX	1	1.037	-2.703	1.69	0.98	2.38	-2.26	2.16	1	1.5042	-1.269	0.01	309.33
GFZ	-0.97	2.8	-1.716	1.87	-1	1.14	0	2	-1	1.852	-0.726	0.01	250.33
IBU	-0.93	2.67	-2.36	2.19	-1	0.85	-0.39	1.96	-0.99	1.71	-1.39	0.01	206.28
LIN	1	-2.27	-0.412	2.85	0.48	-0.6	-2.1	2.88	0.9	-1.33	-1.372	0.05	406.5
MON	-1	3.052	-3.302	1.73	-1	1.49	-1.31	2.24	-0.99	2.12	-2.31	0.02	670.9
NPX	-0.98	1.17	-1.63	1.93	-1	-0.36	0	1.88	-1	0.251	-0.637	0.04	230.6

NFLX	1	-1.07	-1.945	2.24	0.98	-1.01	-2.02	2.72	1	-0.971	-2.064	0.01	319.33
SMZ	-0.092	0.613	-2.78	2.24	-0.91	-0.06	-1.77	2.2	-0.5	0.39	-2.51	0.04	278.33
SULF	-0.41	0.596	-1.97	1.82	-0.99	-0.11	-0.36	1.72	-0.87	0.145	-1.3	0.03	253.28
TCS	-0.02	4.97	-5.27	2.32	-0.68	4.5	-4.79	2.6	-0.17	4.9	-5.193	0.05	289.54
TRIM	0.93	0.269	-1.616	1.96	0.12	1.23	-2.74	2.08	0.59	0.918	-2.415	0.01	290.32
VEN	1	-0.0713	0	1.61	0.89	1.78	-1.62	1.88	0.99	0.836	-0.668	0.01	277.4

^a Net charge off PPCPs in ultrapure water (UPW), synthetic surface water (SSW) and wastewater effluents (WWE) taken from <http://Chemicalize.org> based on their pH (UPW: pH= 6, WWE: pH=7, SSW: pH=8)

^b Dow=pH corrected for Kow, taken from <https://pubchem.ncbi.nlm.nih.gov/>, <http://Chemicalize.org>

^c Solubility, taken from <https://pubchem.ncbi.nlm.nih.gov/>, <http://Chemicalize.org>

^d The nominal concentration for all target compounds were 2 µg L⁻¹. The values reported here are the measured concentrations by LC-MS/MS and has considered uncertainties in the experiments and analytical work

UPW: ultrapure water; SSW: Synthetic river water; WWE: wastewater effluents

Table S10. List of PPCPs, isotopically labeled standard and suppliers

Pharmaceutical	Supplier	Pharmaceutical	Supplier
	r		r
Acetaminophen	Sigma	Gemfibrozil	Sigma
d- Acetaminophen	CDN	d- Gemfibrozil	CDN
Atenolol	Sigma	Ibuprofen	Sigma
d-Atenolol	CDN	d- Ibuprofen	CDN
Atrazine	Sigma	Lincomycin	Sigma
d- Atrazine	CDN	d-Lincomycin	TRC
Atorvastatin	TRC ¹	Naproxen	Sigma
d-Atorvastatin	TRC	d- Naproxen	CDN
d-hydroxy Atorvastatin (o- or 2-)	TRC	Norfluoxetine	Sigma
d-hydroxy Atorvastatin (p- or 4-)	TRC	d-Norfluoxetine	CDN
hydroxy Atorvastatin (o- or 2-)	TRC	Monensin	Sigma
hydroxy Atorvastatin (p- or 4-)	TRC	Sulfamethoxazole	Sigma
Carbamazepine	Sigma	d-Sulfamethoxazole	TRC
d- Carbamazepine	CDN	Sulfamethazine	Sigma ²
10,11epoxide- Carbamazepine	Sigma	d-Sulfamethazine	TRC
d-10,11epoxide- Carbamazepine	CDN	Triclosan	Sigma
Caffeine	CDN	d-Triclosan	CDN ³
d-Caffeine	Sigma	Trimethoprim	Sigma
Diclofenac	Sigma	d- Trimethoprim	CDN
d-Diclofenac	CDN	Venlafaxine	Sigma
Fluoxetine	Sigma	d- Venlafaxine	CDN
d- Fluoxetine	CDN		

¹ Toronto Research Chemicals <https://www.trc-canada.com/>

² Sigma-Aldrich Inc. <https://www.sigmaaldrich.com/canada-english.html>

³ CDN Isotropes https://cdnisotopes.com/ca/?_store=ca_view

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