Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

The degradation and persistence of five pharmaceuticals in artificial climate incubator during one year period

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Sample preparation and instrumental analysis: The last sampling was filtered with a Millipore 0.22µm nylon filter. The transformation products were monitored by high performance liquid chromatography (Ultimate3000 HPLC system, Dionex, USA) coupled to an electrospray ionization tandem mass spectrometry (ESI-MS/MS, API3200, AB Sciex, USA) (HPLC-MS/MS) operated in positive mode. The injection volume was 10 µL. The composition of mobile phase, effect of pH, flow rate and column temperature were optimized to obtain the best chromatographic resolution for simultaneous enantiomeric determination within reasonable analysis time and enough sensitivity for MS spectrometry. The optimized mass spectrometric conditions were as follows: CUR (Curtain Gas) 20 psi, CAD (Collision Gas) 5 psi, IS (Ion Spray Voltage) 5500V, TEM (source temperature) 500^{o}C, GS1 50 psi and GS2 (Ion Source gases) 60 psi. More MS/MS parameters, including declustering potential (DP), collision energy (CE), entrance potential (EP), Collision Cell Entrance Potential (CEP), and collision cell exit potential (CXP), for target TPs are available in Table S3. Concentrations of the detected transformation products have been given in Table S4.

Absorption spectra determination: The solutions of five pharmaceuticals (2 mg L^{-1}) with adjusted pH values 2, 4, 7, 10, and 12 were prepared. The UV-vis absorption spectra of the solutions in the wavelength ranging between 200 nm and 600 nm were determined using Hach DR-5000 UV-Vis spectrophotometer.

Table S1 The quantum chemistry descriptors used to develop the equation (3)

Compounds	HOF[a]	E_{HOMO}[b]	E_{LUMO}[c]	TE[d]	E_{LUMO}-E_{HOMO}
ATN	-545.23	-9.13	-0.148	-3275.71	8.98
MTP	-522.03	-8.81	0.136	-3251.98	8.94
PHO	-136.25	-8.03	-0.721	-3024.23	7.31
FLX	-644.61	-8.76	-0.426	-4209.61	8.33
VFX	-353.38	-8.28	0.68	-3229.42	8.96

[a]: heat of formation in kJ/mol

[b]: the energy of the highest occupied molecular orbital in eV

[c]: the energy of the lowest unoccupied molecular orbital in eV[d]: total energy in eV

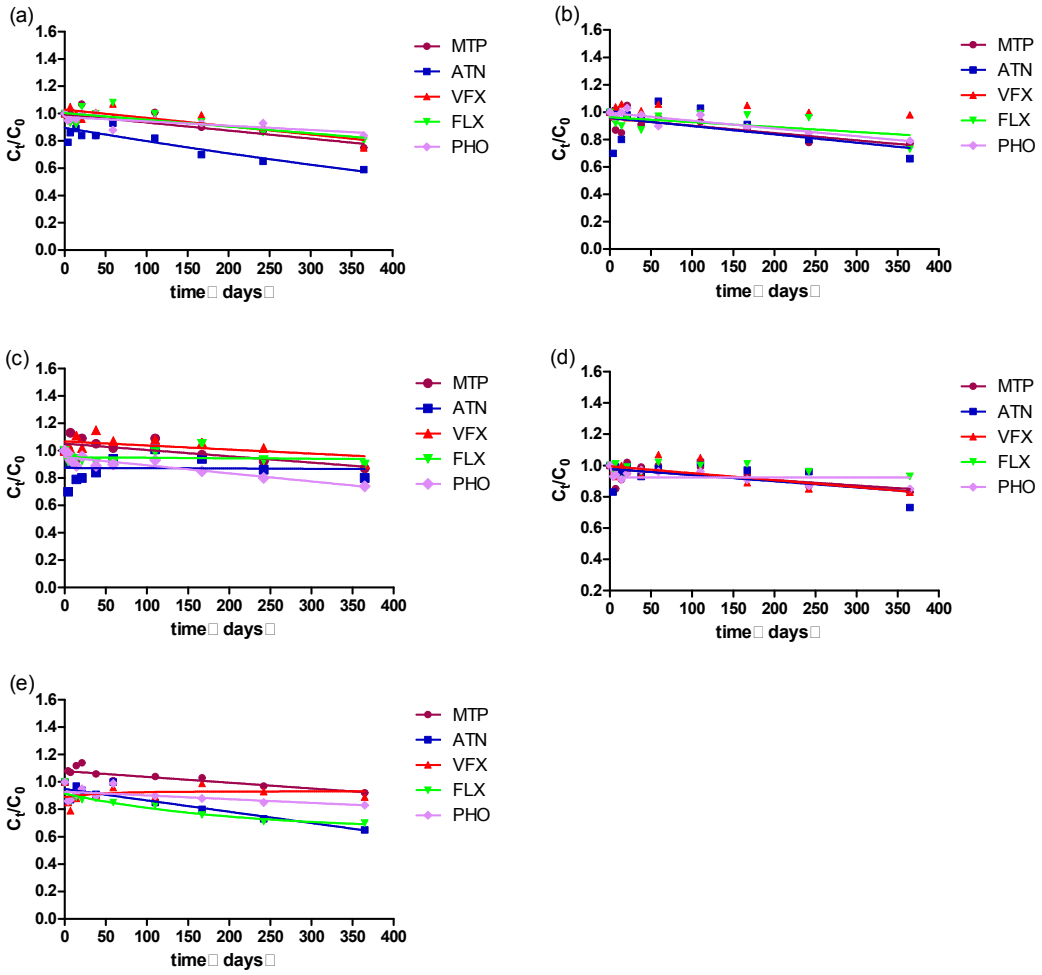

Fig.S1 The effect of pH values on the degradation for atenolol, metoprolol, propranolol, fluoxetine, venlafaxine at (a) pH=2, (b) pH=4, (c) pH=7, (d) pH=10, (e) pH=12 in water in the dark

Table S2 Physicochemical properties of main transformation products

transformation product	Formula	Parent compound	MW (g/mol)	pKa	logKow	Ref
metoprolol acid	$C_{14}H_{21}NO_4$	Atenolol	267	9.7	-4.17	1
α-hydroxymetoprolol	$C_{15}H_{25}NO_4$	Metoprolol	284	9.7	0.84	2
4- hydroxypropranolol	$C_{16}H_{21}NO_3$	Propranolol	275	--	2.81	3
norfluoxetine	$C_{16}H_{16}F_3NO$	Fluoxetine	295	9.37	n/a	4
desmethylvenlafaxine	$C_{16}H_{25}NO_2$	Venlafaxine	263	9.74	0.74	4

MW, molecular weight; pKa, dissociation constant; logKow, partition coefficient (Octanol/water); n/a , not available.

Table S3 the MS/MS parameters (declustering potential (DP), collision energy (CE), entrance potential (EP), Collision Cell Entrance Potential (CEP), collision cell exit potential (CXP)) for target TPs

TPs	Q1 (m/z)	Q3 (m/z)	DP (V)	EP (V)	CEP (V)	CE (eV)	CXP (V)
metoprolol acid	268.2	145.2	46	5	16	25	8
α-hydroxymetoprolol	284.2	74.1	51	4	16	30	8
4- hydroxypropranolol	276.1	173.2	46	6	14	27	4
norfluoxetine	296.1	134.2	16	4	18	9.8	3
desmethylvenlafaxine	264.2	58.1	31	5.5	14	28	8

Table S4 Concentrations of four transformation products the last sampling (after one year) under fluorescent lamp

Compounds	Concentration(μg/L)									
	pH=2		pH=4		pH=7		pH=10		pH=12	
	E_1	E_2	E_1	E_2	E_1	E_2	E_1	E_2	E_1	E_2
metoprolol acid	12	16	370	308	636	638	801	700	724	661
α-hydroxymetoprolol	76	69	53	49	-	-	-	-	-	-
norfluoxetine	-	-	-	-	-	-	25	30	60	50
desmethylvenlafaxine	44	48	18	21	14	15	6	6	-	-

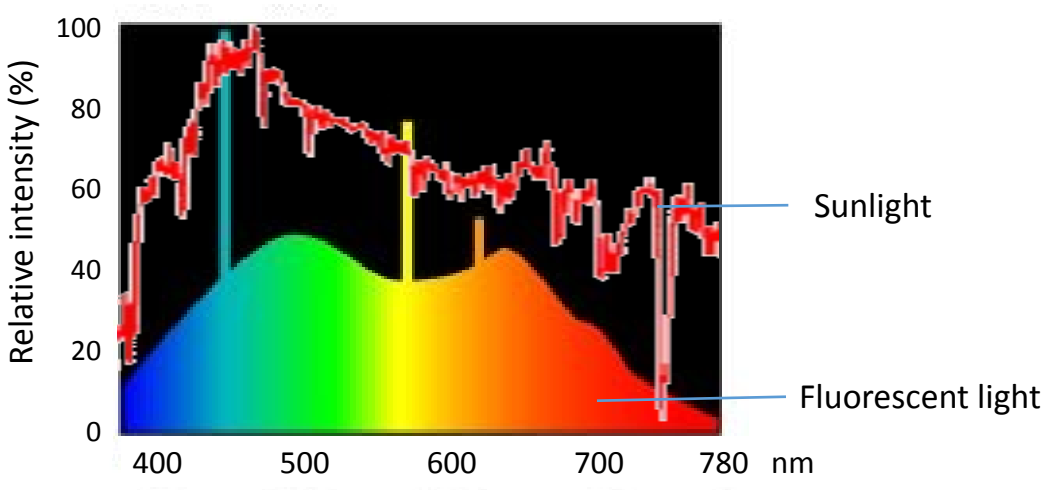

Figure S2 The spectrum of fluorescent light and sunlight

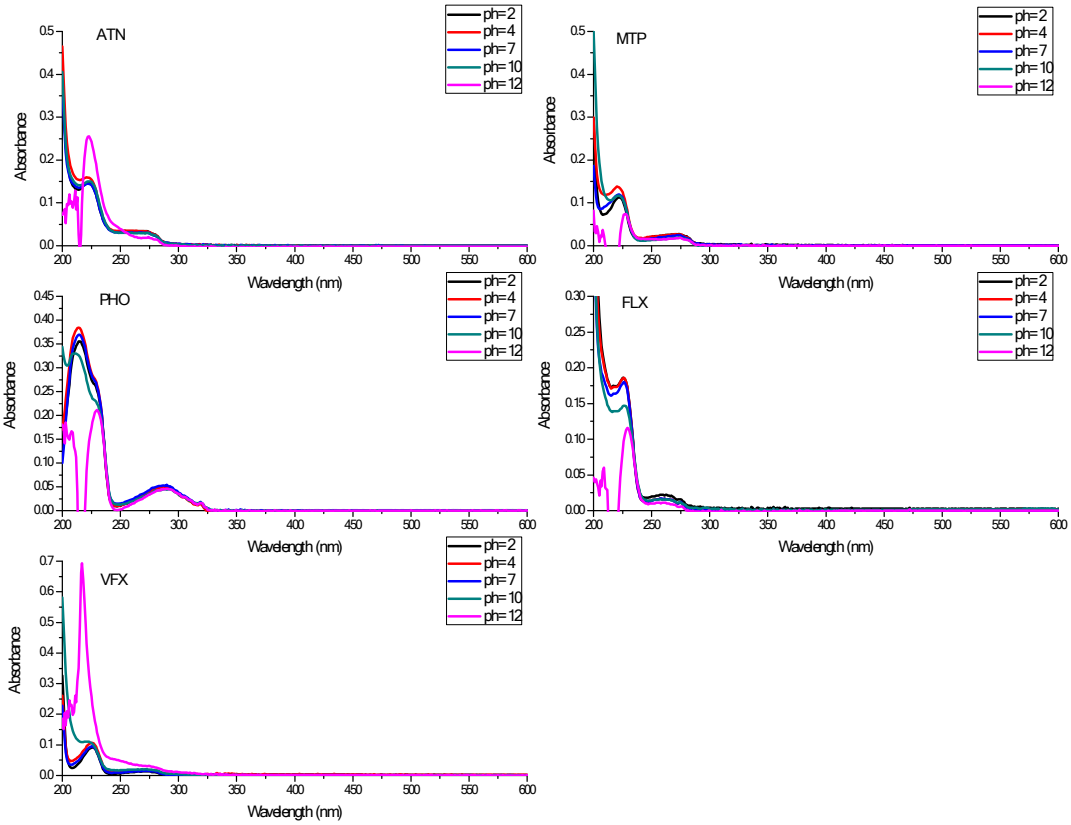

Fig. S3 Absorption spectra of the five pharmaceuticals under different pH values

Reference

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