Supplementary materials

Photocatalytic degradation of the antidepressant drug Paroxetine using TiO_2 P-25 under lab and pilot scales in aqueous substrates

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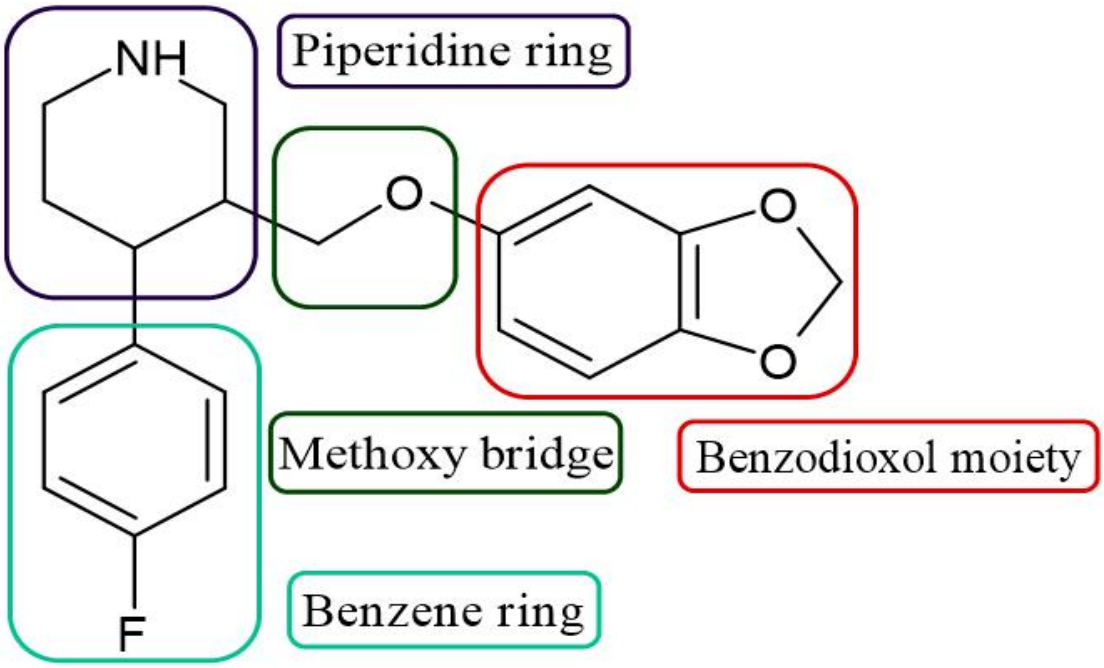

Supplementary Figure 1. PXT chemical formula.

Supplementary Figure 2. The CPC pilot plant placed at the WWTP of the University Hospital of Ioannina.

Reagents, solvents, and materials

Acetonitrile (ACN) and water solvents (HPLC grade), and water, methanol solvents (LC-MS grade) were provided by Fisher Scientific (Loughborough, UK). Formic Acid (FA) LC-MS grade was supplied by Carlo Erba (Barcelona, Spain). Hydrochloric acid (HCl) (37%, *v/v*) was supplied by Merck (Darmstadt, Germany). Sodium Carbonate (Na_2CO_3) (≥ 99%), *para*-hydroxy-benzoic acid (99%), and sodium hydroxide were purchased from Sigma-Aldrich (St. Louis, MO, USA). Bis (2-hydroxyethyl) amino-tris (hydroxymethyl) methane (Bis-Tris), sodium nitrite ($NaNO_2$), disodium ethylenediaminetetraacetate (Na_2EDTA), Folin-Ciocalteu's reagent and PVDF Durapore filtering membranes (0.45 μm pore diameter) were supplied by Merck (Darmstadt, Germany). Boric Acid (H_3BO_3) was purchased from Supelco (Bellefonte, PA, USA), sodium Nitrate ($NANO_3$) was purchased from Fluka (Buchs, Switzerland), and sodium fluoride (NaF) was purchased from Penta (Prague, Czech Republic). OASIS solid phase extraction cartridges (200 mg, 6 mL) were supplied by Waters Corporation (Milford, MA, USA), while HLB^+ micro-cartridges (60 mg, 3 mL) were supplied by Chromatific (Heidenrod, Germany).

Supplementary Table 1. Minimum (min), maximum (max), standard deviation (s.d.), and median values of the physicochemical parameters of secondary treated HWW

Parameter	Min	Max	S.D.	Median
Conductivity (μS/cm)	1060	1959	300.9	1305
pH	6.2	7.4	0.29	6.8
TOC (mg/L)	3.38	34.50	9.48	10.46
TDS (mg/L)	389	1108	419.8	414
BOD_5 (mg/L)	7.00	47.90	15.11	5.60
COD (mg/L)	<10	142.0	43.94	0.84
Abs_{254}	0.16	0.18	0.01	0.17
Total Phenols (mg/L)	0.66	1.62	0.33	0.98
Cl^- (mg/L)	121.8	357.0	90.40	218.9
NO_3^- (mg/L)	51.42	119.4	25.61	56.85
SO_4^{2-} (mg/L)	20.80	43.10	8.35	28.92

Supplementary Table 2. Operational parameters of the LTQ-ORBITRAP instrumentation

Parameter	Value
Resolution	60,000 FWHM
Full Scan	50 – 800 Da
Mass Tolerance	≤ 5 ppm
Sheath Gas	35 a.u.
Auxiliary Gas flow	10 a.u.
Spray Voltage	3,7 kV
Collision Energy	35 eV
Capillary Voltage	50 V
Capillary Temperature	320 °C
Tube Lens	90 V

Supplementary Table 3. Pseudo-first order rate constants (k_{app}), correlation coefficient (R^2), and half-life time ($t_{1/2}$) of PXT after lab-scale photocatalytic treatment.

TiO_2 P-25	PXT (10 mg/L)		
C (mg/L)	k_{app} (min^{-1})	R^2	$t_{1/2}$ (min)
200	0.074	0.9904	9.367
300	0.079	0.9780	8.774
500	0.092	0.9726	7.534

Supplementary Table 4. Pseudo-first order rate constant (k_{app}), correlation coefficient (R^2), and half-life time ($t_{1/2}$) of TOC decrease after lab-scale photocatalytic treatment

TiO_2 P-25	TOC		
C (mg/L)	k_{app} (min^{-1})	R^2	$t_{1/2}$ (min)
200	0.003	0.9080	231.05
300	0.006	0.9823	115.52
500	0.007	0.9829	99.021