Supplementary Materials for the Article:

Identification of photodegradation products of escitalopram in surface water by HPLC-MS/MS and preliminary characterization for their potential impact on the environment

Veronica Termopoli[1], Viviana Consonni[1], Davide Ballabio[1], Roberto Todeschini[1], Marco Orlandi[1], and Fabio Gosetti[1,*]

[1] Department of Earth and Environmental Sciences (DISAT), University of Milano-Bicocca, Piazza della Scienza 1, 20126 Milano, Italy

* Correspondence: fabio.gosetti@unimib.it

Table S1. Selected Reaction Monitoring transitions of the HPLC-MS/MS method for ESC and TPs monitoring.

Precursor ion $[M+H]^+$ ***m/z***	**Product ions** ***m/z***
245	200 /227
247	229 /202
261	216/243
311	109/262
323	260/109
325	109/262
327	309/109
337	274/294
339	276/258
341	262/109
343	237/109
355	294/337
357	339/321

Table S2. *In silico* prediction of ecotoxicity, mutagenicity, bioaccumulation and persistence of ESC and its TPs by VEGA [44] and T.E.S.T. [45] software

ID	SMILES	ToxFish[1]	ToxDaph[2]	ToxTpyr[3]	ToxRat[4]	Ames[5]	ToxDev[6]	Biodeg[7]	BCFmAG[8]	PerWat[9]	PerSed[10]	PerSoil[11]
ESC	C[NH+](C)CCC[C@]2(OCc1cc(ccc12)C#N)c3ccc(F)cc3	0.29	3.90	4.70	688.7	-	+	nonRB*	2.44	23	157	23
TP1	C[NH+](C)CCC(O)C2OC(=O)c1cc(ccc12)C#N	1.96	5.30	47.48	418.8	-	+	nonRB	0.09	7	23	34
TP2	C[NH+](C)CCCC2OC(=O)c1cc(ccc12)C#N	1.85	1.73	24.33	536.9	-	+	nonRB	0.63	7	23	34
TP3	C[NH+](C)CC(O)C[C@]2(OC(O)c1cc(ccc12)C#N)c3ccc(F)cc3	0.46	1.63	17.51	447.9	-	+	nonRB	0.98	26	227	26
TP4	C[NH+](C)CCCC2(O)OCc1cc(ccc12)C#N	14.51	6.62	68.73	466.9	+	+	nonRB	0.86	4	227	20
TP5	Oc1ccc(cc1)[C@]3(CCC[NH+](C)C)OC(=O)c2cc(ccc23)C#N	0.36	1.88	4.21	580.2	-	+	nonRB	1.02	7	227	26
TP6	C[NH2+]CC(O)C[C@]2(OCc1cc(ccc12)C#N)c3ccc(F)cc3	0.64	4.41	14.18	1013.3	-	+	nonRB	2.20	26	157	34
TP7	C[NH+](C)CCC[C@]2(OCc1cc(ccc12)C#N)c3ccc(O)cc3	0.48	1.60	5.91	646.2	-	+	nonRB	1.53	23	227	26
TP8	NC(=O)c1ccc2c(c1)CO[C@@]2(CCC[NH+](C)C)c3ccc(F)cc3	1.57	5.03	22.03	752.4	-	+	nonRB	1.44	23	227	23
TP9	C[NH+](C)CC(O)C[C@]2(OCc1cc(ccc12)C#N)c3ccc(F)cc3	0.39	3.64	12.49	717.9	-	+	nonRB	1.67	26	157	23
TP10	C[NH+](CO)CC(O)C[C@]2(OCc1cc(ccc12)C#N)c3ccc(F)cc3	0.37	8.00	76.97	399.1	+	+	nonRB	1.00	26	157	26
TP11	C[NH2+]CCC(O)[C@]2(OCc1cc(ccc12)C#N)c3ccc(F)cc3	0.39	4.74	14.44	537.7	-	+	nonRB	2.20	26	227	34
TP12	C[NH+](C)CCC(O)[C@]2(OCc1cc(ccc12)C#N)c3ccc(F)cc3	0.40	3.93	12.73	657.5	-	+	nonRB	1.67	26	227	94
TP13	C[NH+](C)CC(O)C[C@]2(OC(=O)c1cc(ccc12)C#N)c3ccc(F)cc3	0.12	2.28	7.10	678.1	-	+	nonRB	1.17	7	157	23
TP14	Fc1ccc(cc1)[C@]3(CCC[NH+](C)C)OC(=O)c2cc(ccc23)C#N	0.25	0.47	3.15	545.9	-	+	nonRB	1.91	7	157	23
TP15	Fc1ccc(cc1)[C@]3(CCC[NH2+]C)OCc2cc(ccc23)C#N	0.33	1.15	4.91	1011.3	-	+	nonRB	3.19	23	157	34
TP16	Fc1ccc(cc1)[C@@]3([OH+]Cc2cc(ccc23)C#N)CCCN(C)(C)=O	0.08	0.50	6.91	475.9	-	+	nonRB	3.25	23	23	34

[1] Acute Toxicity Fish (Fathead minnow LC50 (96 h)), mg/L, CONSENSUS model, T.E.S.T.

[2] Daphnia magna LC50 (48 h), mg/L, CONSENSUS model,T.E.S.T.

[3] T. pyriformis IGC50 (48 h), mg/L, CONSENSUS model,T.E.S.T.

[4] Oral rat LD50, mg/kg, CONSENSUS model,T.E.S.T.

[5] Mutagenicity (Ames test) CONSENSUS model (version 1.0.4), VEGA

[6] Developmental Toxicity model (CAESAR) (version 2.1.8), VEGA

[7] Ready Biodegradability model (IRFMN) (version 1.0.10), VEGA

[8] BCF model (Arnot-Gobas) (version 1.0.1), log(BCF), VEGA

[9] Persistence (water) quantitative model (IRFMN) (version 1.0.1) days, VEGA

[10] Persistence (sediment) quantitative model (IRFMN) (version 1.0.1) days, VEGA

[11] Persistence (soil) quantitative model (IRFMN) (version 1.0.1) days, VEGA

* nonRB = non Readily Biodegradable

Table S3. *Results of matrix effect (ME) evaluation*

Calibration plot in the range between LOQ and 2.5 ng/mL				
	External calibration		*Standard Addition*	
	Concentration level	Average peak area	Concentration level	Average peak area
	0.01	1476.39	0.01	272.65
	0.05	5633.74	0.05	5174.61
	0.1	11465.08	0.1	9078.33
	0.5	52097.56	2.5	279854.9
	1	105538.38		
	2.5	276744.69		
Equation	*y = (108396.9 ± 1505.5)x*		*y = (111989.5 ± 1978.9)x*	
Calibration plot in the range between 2.5 and 1000 ng/mL				
	External calibration		*Standard Addition*	
	Concentration level	Average peak area	Concentration level	Average peak area
	2.5	276744.69	5	225143.50
	10	605115.56	10	555707.31
	25	1614979.14	25	1369777.11
	50	3049573.26	50	2948505.14
	100	5710348.12	100	5766037.52
	250	15031543.08	250	15026532.57
	500	29901912.87	500	23468441.51
	1000	62626401.17	1000	58622435.74
Equation	*y = (60976.6 ± 827.2)x*		*y = (55752.3 ± 2236.5)x*	

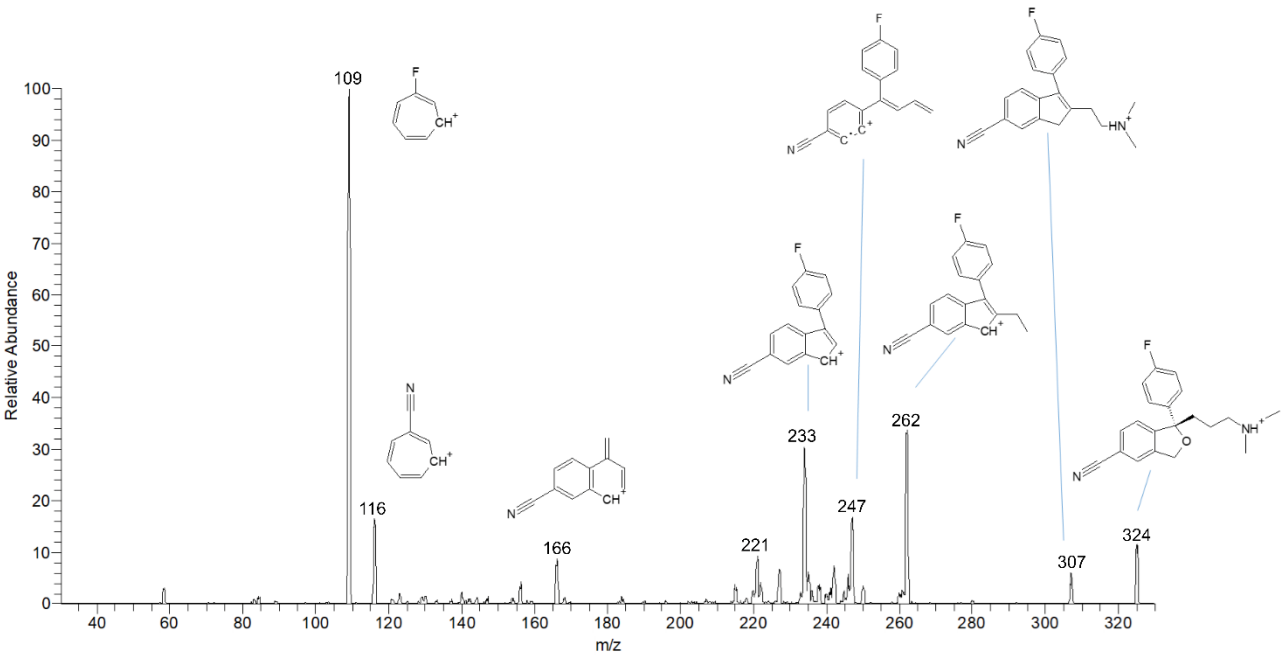

Figure S1. MS/MS spectrum of ESC with the chemical structures of the product ions

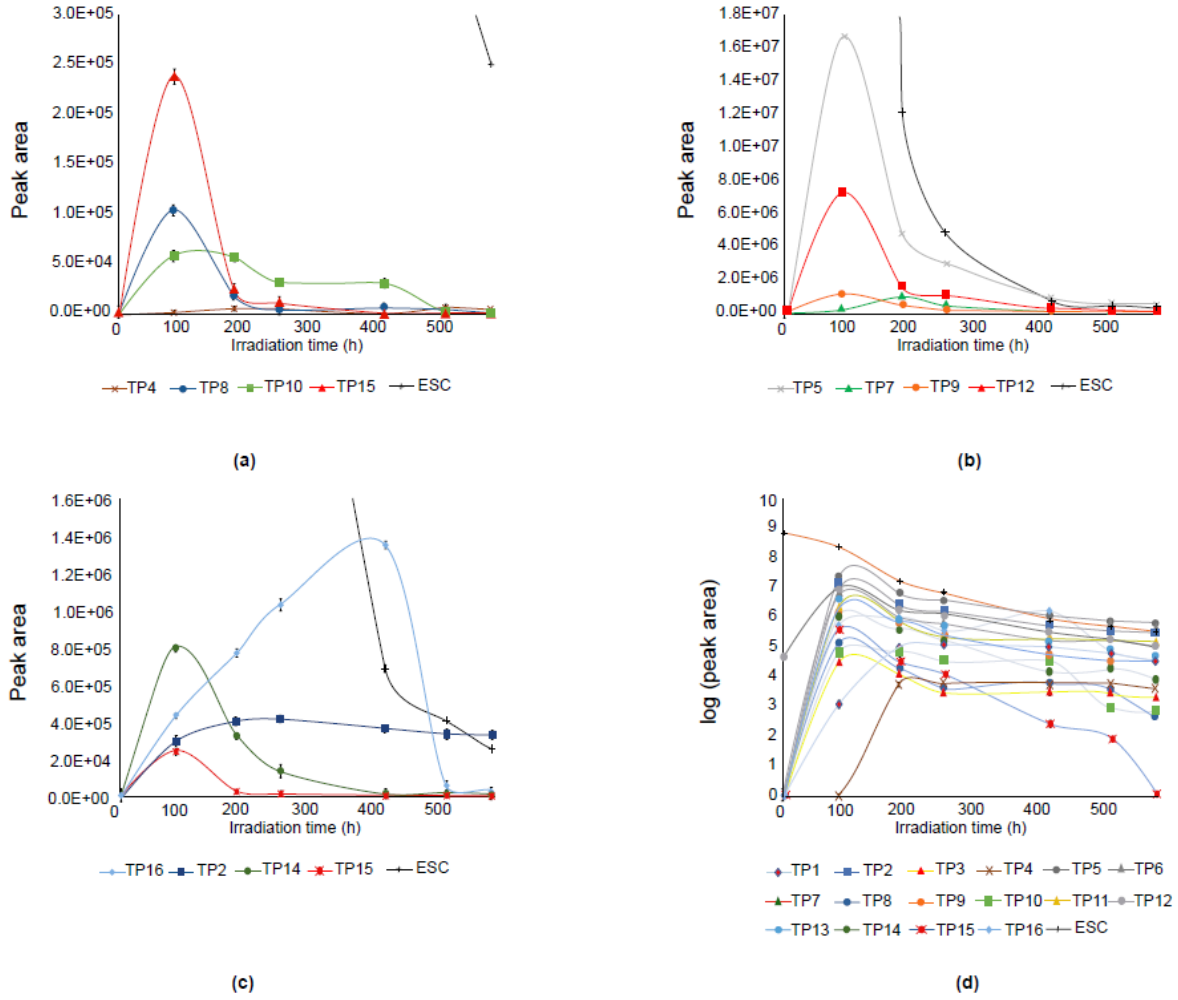

Figure S2. Time evolution of the peak areas of TPs formed during the ESC photodegradation

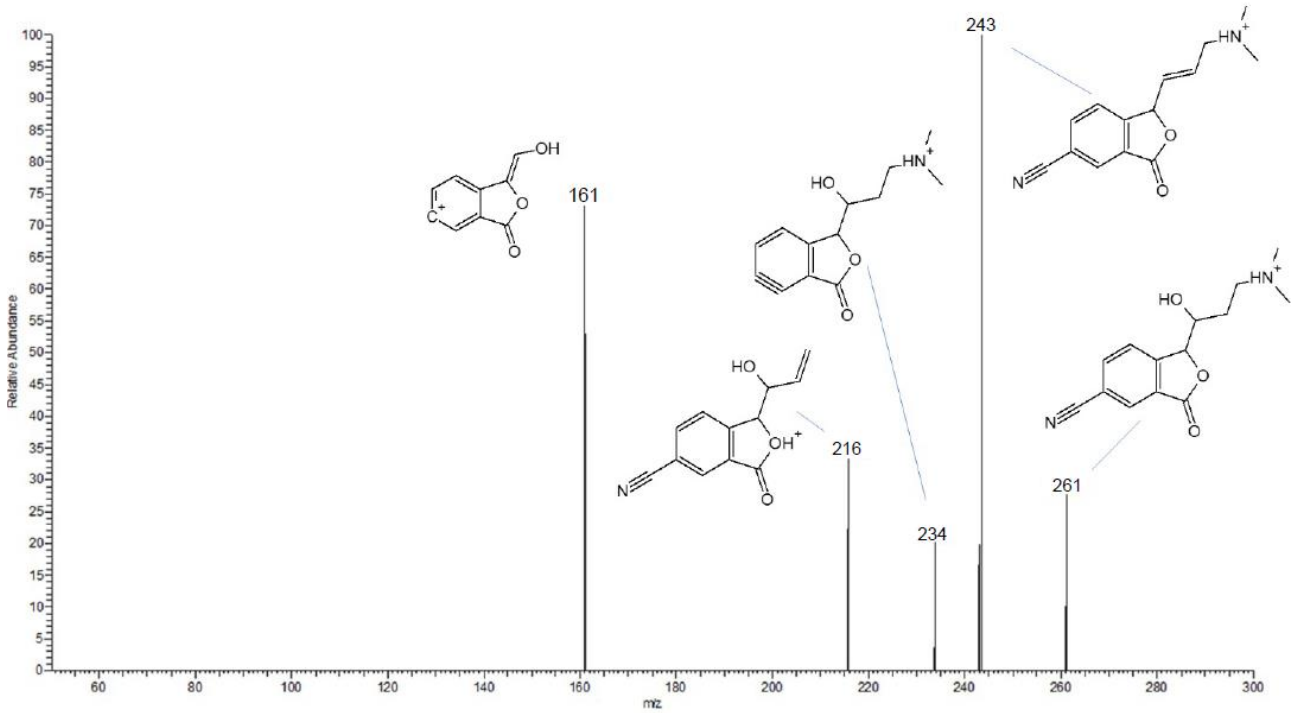

Figure S3. MS/MS spectrum of TP1 at *m/z* 261 with the chemical structures of the product ions

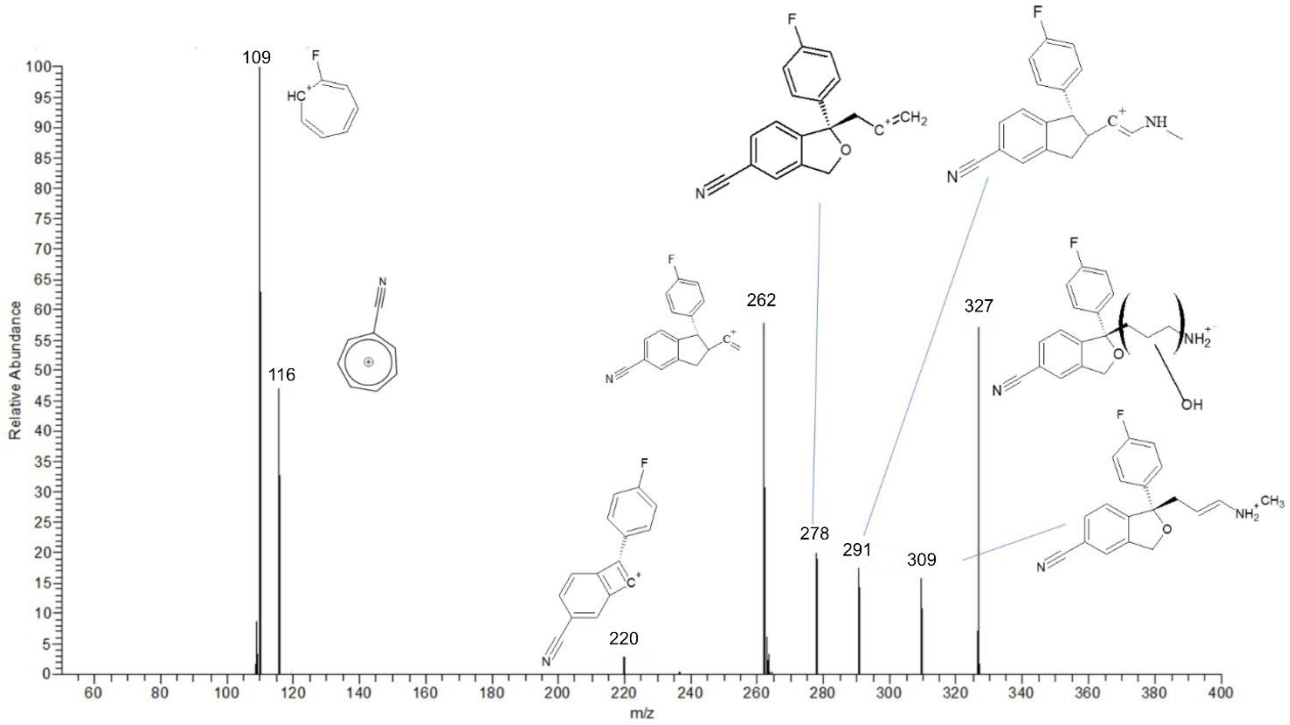

Figure S4. MS/MS spectrum of TP6 at *m/z* 327 with the chemical structures of the product ions

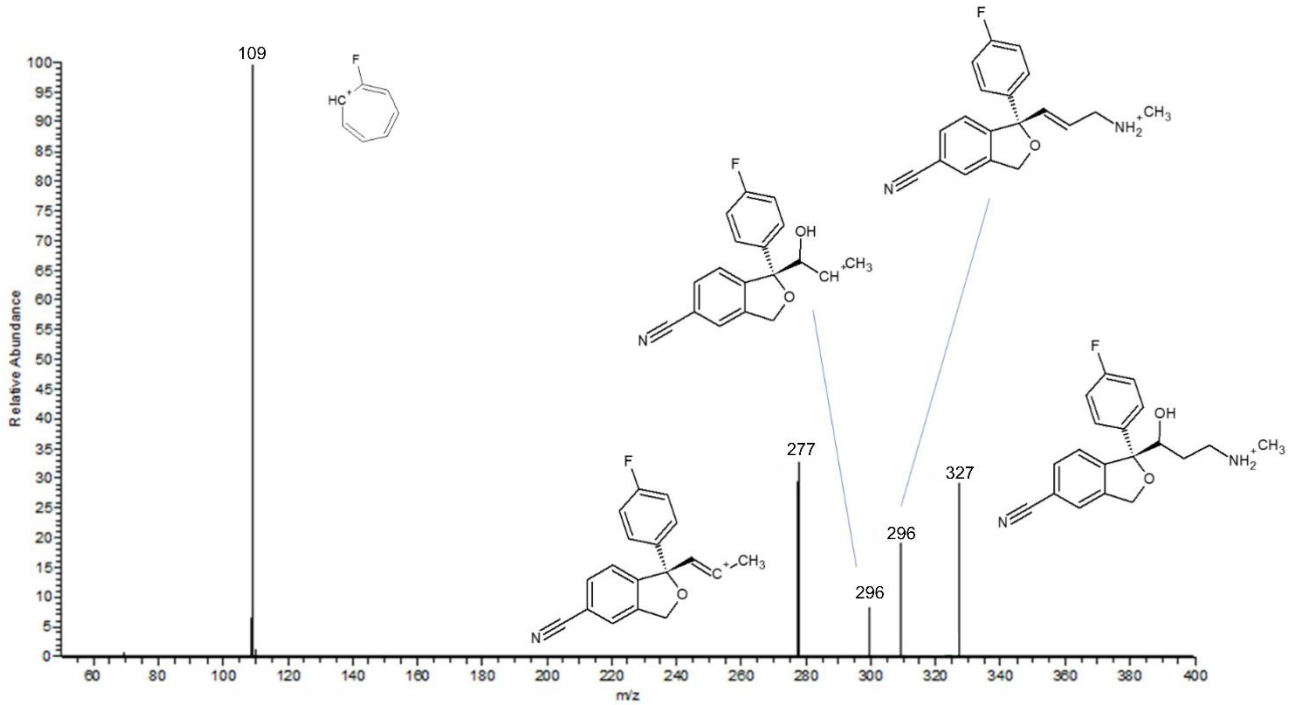

Figure S5. MS/MS spectrum of TP11 at *m/z* 327 with the chemical structures of the product ions