

SUPPLEMENTARY MATERIAL

Table S1 Half-life time (min) for the investigated pollutants in mixture (2 mg/L each, 1000 mg/L of catalyst)

	Milli-Q Water			Wastewater		
	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG
Carbamazepine	7.30	3.57	3.40	8.45	6.42	6.36
Sulfamethoxazole	5.98	1.96	3.04	9.12	5.73	7.30
Atenolol	6.93	3.89	3.87	7.15	6.60	5.82
Bisphenol A	4.15	4.10	3.21	4.15	5.33	10.05
Diclofenac	4.92	5.78	4.62	7.45	5.92	5.25
Caffeine	5.73	4.18	5.55	7.97	5.50	7.15
Ibuprofen	2.36	1.79	1.62	13.33	5.37	5.42

Table S2 TPs formed from CBZ degradation in wastewater (mean peak areas).

TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG	TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG
287 A	1.34x10 ⁵	6.90x10 ⁵	-	269 A	1.00x10 ⁵	1.66x10 ⁵	1.21x10 ⁵
287 B	1.50x10 ⁶	3.60x10 ⁶	-	269 B	1.64x10 ⁵	5.98x10 ⁵	3.32x10 ⁵
271 A	4.12x10 ⁵	1.06x10 ⁶	1.33x10 ⁵	269 C	1.79x10 ⁵	4.52x10 ⁵	7.18x10 ⁵
271 B	9.76x10 ⁵	1.37x10 ⁶	1.36x10 ⁴	269 D	1.49x10 ⁵	7.27x10 ⁴	3.54x10 ⁵
267 A	6.42x10 ⁴	4.97x10 ⁴	4.81x10 ⁵	253 A	1.26x10 ⁶	1.78x10 ⁶	7.46x10 ⁶
267 B	2.26x10 ⁵	1.32x10 ⁵	1.91x10 ⁶	253 B	7.22x10 ⁶	9.03x10 ⁶	4.00x10 ⁷
267 C	1.25x10 ⁵	5.95x10 ⁴	6.49x10 ⁵	253 C	9.55x10 ⁶	1.14x10 ⁷	4.77x10 ⁷
267 D	7.09x10 ⁴	6.14x10 ⁴	1.65x10 ⁵	253 D	1.25x10 ⁶	9.70x10 ⁶	7.00x10 ⁶
267 E	7.04x10 ⁴	1.70x10 ⁵	1.82x10 ⁴	251	5.51x10 ⁶	1.73x10 ⁶	1.63x10 ⁷
226	2.40x10 ⁵	-	9.50x10 ⁵	224	3.94x10 ⁵	1.08x10 ⁶	9.04x10 ⁶
223	4.13x10 ⁵	1.00x10 ⁶	1.59x10 ⁶				

Table S3 TPs formed from SMX degradation in wastewater (mean peak areas).

TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG	TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG
288	1.20x10 ⁴	1.84x10 ⁵	4.10x10 ⁵	172	5.48x10 ⁴	1.10x10 ⁵	8.83x10 ⁴
286 B	2.87x10 ⁴	2.58x10 ⁵	4.86x10 ⁵	156	6.31x10 ⁵	5.86x10 ⁵	9.55x10 ⁵
284	1.14x10 ⁵	-	2.40x10 ⁵	110	7.39x10 ⁴	1.09x10 ⁵	-
270 A	5.22x10 ⁴	1.63x10 ⁵	7.30x10 ⁵	108	5.77x10 ⁴	1.60x10 ⁵	3.10x10 ⁵
270 B	7.89x10 ⁶	2.15x10 ⁷	3.38x10 ⁶				

Table S4 TPs formed from ATL degradation in wastewater (mean peak areas).

TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG	TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG
315 C	2.47x10 ⁴	2.83x10 ³	2.24x10 ⁴	281 A	7.59x10 ³	2.91x10 ⁴	4.34x10 ⁴
315 D	2.89x10 ⁴	6.75x10 ⁴	2.94x10 ⁵	281 B	1.45x10 ⁵	5.94x10 ⁴	9.46x10 ⁵
315 F	4.37x10 ⁵	5.99x10 ⁵	3.64x10 ⁶	254	8.50x10 ⁴	5.11x10 ⁴	4.82x10 ⁵
297	2.03x10 ⁵	8.68x10 ⁵	3.22x10 ⁶	238	8.60x10 ⁵	5.57x10 ⁷	7.01x10 ⁶
283 B	1.12x10 ⁵	2.38x10 ⁵	2.13x10 ⁶	225	1.88x10 ⁴	6.68x10 ⁴	1.98x10 ⁵
283 C	4.33x10 ⁵	-	5.65x10 ⁵	152	5.44x10 ⁵	6.26x10 ⁵	4.34x10 ⁶
283 D	7.95x10 ⁵	2.94x10 ⁶	4.22x10 ⁶	134	1.50x10 ⁷	5.78x10 ⁸	7.89x10 ⁷
283 E	7.70x10 ³	2.39x10 ⁵	8.91x10 ⁵	232	7.48x10 ⁴	9.19x10 ⁴	7.41x10 ⁵
283 F	-	2.85x10 ⁴	1.54x10 ⁵				

Table S5 TPs formed from BPA degradation in wastewater (mean peak areas).

TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG	TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG
273	1.12x10 ⁵	7.74x10 ⁴	3.11x10 ⁵	165	4.77x10 ³	3.57x10 ⁴	-
257	2.23x10 ⁴	7.11x10 ⁴	7.20x10 ⁵	151	4.58x10 ⁴	-	3.22x10 ⁴
243 A	2.92x10 ⁴	1.66x10 ⁵	4.43x10 ⁴	135	6.43x10 ⁴	-	2.88x10 ⁵
243 B	2.77x10 ³	7.35x10 ²	6.47x10 ⁴				

Table S6 TPs formed from DCF degradation in wastewater (mean peak areas).

TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG	TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG
324	2.4x10 ³	2.13x10 ⁴	-	276	4.53x10 ³	1.20x10 ⁴	4.42x10 ⁴
310 A	4.43x10 ⁴	3.11x10 ⁴	2.07x10 ⁴	264	3.88x10 ⁴	6.48x10 ⁴	3.52x10 ⁵
310 B	2.57x10 ⁵	1.99x10 ⁵	1.33x10 ⁶	150	7.34x10 ⁴	8.92x10 ³	1.52x10 ⁵

Table S7 TPs formed from IBP degradation in wastewater (mean peak areas).

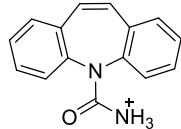
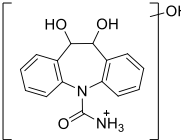
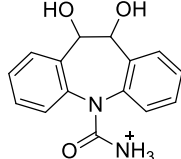
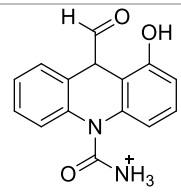
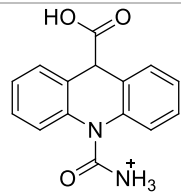
TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG	TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG
267 A	-	-	4.73x10 ³	237 C	3.26x10 ³	8.48x10 ⁴	1.39x10 ⁶
267 B	7.24x10 ³	2.58x10 ⁴	4.52x10 ⁵	221 A	-	-	2.19x10 ⁵
253 A	-	2.25x10 ⁴	2.14x10 ⁴	221 B	-	-	1.97x10 ⁵
253 B	-	-	3.92x10 ⁴	221 C	-	-	7.18x10 ⁴
253 C	-	-	5.17x10 ⁴	221 D	-	3.32x10 ⁴	3.21x10 ⁴
253 D	-	1.35x10 ⁴	6.24x10 ⁴	221 E	1.62x10 ⁶	1.45x10 ⁶	2.77x10 ⁶
251 A	2.38x10 ⁵	2.41x10 ⁴	1.69x10 ⁶	219	-	-	1.59x10 ⁵
251 B	3.16x10 ⁵	6.54x10 ⁴	2.74x10 ⁶	207	-	-	1.06x10 ⁵
237 A	1.70x10 ⁴	7.30x10 ⁴	1.18x10 ⁶	191 B	2.72x10 ³	3.83x10 ⁴	9.54x10 ⁴
237 B	3.79x10 ³	7.74x10 ⁴	1.49x10 ⁶	177	-	1.03x10 ³	5.81x10 ³

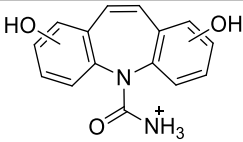
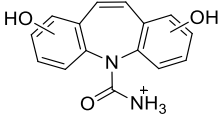
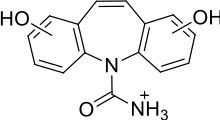
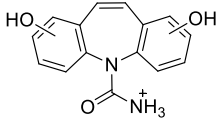
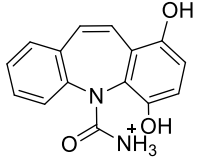
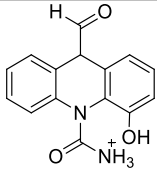
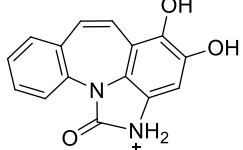
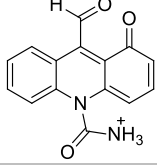
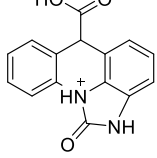
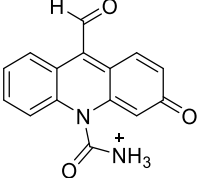
Table S8 TPs formed from CAF degradation in wastewater (mean peak areas).

TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG	TP	TiO ₂ -P25	Ce-ZnO	TiO ₂ -SG
229	5.12x10 ⁵	6.94x10 ⁵	6.87x10 ⁵	170 B	-	3.20x10 ⁵	5.65x10 ⁵
213	8.95x10 ⁵	2.24x10 ⁵	4.11x10 ⁵	144	2.98x10 ⁴	8.83x10 ⁵	1.12x10 ⁶
201 A	3.43x10 ⁶	1.46x10 ⁶	1.10x10 ⁶	142 A	1.69x10 ⁵	1.97x10 ⁶	4.53x10 ⁶
201 B	-	1.97x10 ⁵	3.12x10 ⁵	142 B	1.12x10 ⁵	9.49x10 ⁴	1.30x10 ⁶
199 A	3.48x10 ⁵	2.64x10 ⁵	1.51x10 ⁵	128	2.56x10 ⁶	3.19x10 ⁵	2.78x10 ⁵
199 B	-	6.54x10 ⁴	5.83x10 ⁴	127	1.84x10 ⁵	8.57x10 ⁶	7.53x10 ⁶
199 C	9.53x10 ⁴	8.84x10 ⁴	1.49x10 ⁵	118	5.63x10 ⁴	8.94x10 ⁶	3.57x10 ⁵
184	2.14x10 ⁵	5.51x10 ⁵	7.75x10 ⁵	103	6.64x10 ⁵	4.85x10 ⁶	3.39x10 ⁶
170 A	1.89x10 ⁴	5.49x10 ⁵	2.34x10 ⁵				

Tables S9-S13 show the transformation products detected during the photodegradation of investigated CECs (10 mg/L) with TiO₂ (200 mg/L) in MilliQ water, with the proposed formula and the references used for the identification of the different TPs.

Table S9. Carbamazepine

Precursor ion [M+H] ⁺	t _R (min)	Product ions		Structure	Ref.
		MS ²	MS ³		
CBZ 237.1025 C₁₅H₁₃ON₂	20.81	194.0965 C ₁₄ H ₁₂ N (-CHON) [100]	-		[1]
		220.07605 C ₁₅ H ₁₀ NO ⁺ (-NH ₃) [1.08]	-		
287.1031 C₁₅H₁₅O₄N₂⁺	A 11.57	269.0958 C ₁₅ H ₁₃ O ₃ N ₂ (-H ₂ O) [100]	226.0860 C ₁₄ H ₁₂ O ₂ N (-CHON) [100] 252.0655 C ₁₅ H ₁₀ O ₃ N (-NH ₃) [95] 196.0755 C ₁₃ H ₁₀ ON (-C ₂ H ₃ O ₂ N) [11]		[1]
	B 12.74	269.0959 C ₁₅ H ₁₃ O ₃ N ₂ (-H ₂ O) [100]	226.0861 C ₁₄ H ₁₂ O ₂ N (-CHON) [100] 252.0655 C ₁₅ H ₁₀ O ₃ N (-NH ₃) [95] 196.0753 C ₁₃ H ₁₀ ON (-C ₂ H ₃ O ₂ N) [11]		
	C 14.99	269.0958 C ₁₅ H ₁₃ O ₃ N ₂ (-H ₂ O) [100]	252.0653 C ₁₅ H ₁₀ O ₃ N (-NH ₃) [100] 196.0753 C ₁₃ H ₁₀ ON (-C ₂ H ₃ O ₂ N) [58] 226.0857 C ₁₄ H ₁₂ O ₂ N (-CHON) [29.5]		
		226.0893 C ₁₄ H ₁₂ O ₂ N (-CH ₃ O ₂ N) [3.5]	-		
271.1083 C₁₅H₁₅O₃N₂⁺	A 10.80	253.1008 C ₁₅ H ₁₃ O ₂ N ₂ (-H ₂ O) [100]	236.0701 C ₁₅ H ₁₀ O ₂ N (-NH ₃) [100] 210.0908 C ₁₄ H ₁₂ ON(-CHON) [57] 180.0801 C ₁₃ H ₁₀ N (-C ₂ H ₃ O ₂ N) [16] 208.0752 C ₁₄ H ₁₀ ON (-CH ₃ ON) [6]		[1]
		236.0739 C ₁₅ H ₁₀ O ₂ N (-H ₅ ON) [8.5]	-		
		210.0941 C ₁₄ H ₁₂ ON (-CH ₃ O ₂ N) [5]	-		
	B 14.24	253.1009 C ₁₅ H ₁₃ O ₂ N ₂ (-H ₂ O) [100]	236.0701 C ₁₅ H ₁₀ O ₂ N (-NH ₃) [100] 210.0908 C ₁₄ H ₁₂ ON(-CHON) [57] 180.0801 C ₁₃ H ₁₀ N (-C ₂ H ₃ O ₂ N) [16] 208.0752 C ₁₄ H ₁₀ ON (-CH ₃ ON) [5]		
		236.0741 C ₁₅ H ₁₀ O ₂ N (-H ₅ ON) [8.5]	-		
		210.0940 C ₁₄ H ₁₂ ON(-CH ₃ O ₂ N) [5]	-		
269.0926 C₁₅H₁₃O₃N₂⁺	A 11.57	226.0859 C ₁₄ H ₁₂ O ₂ N (-CHON) [100]	198.0907 C ₁₃ H ₁₂ ON (-CO) [100]		[1]
		252.0653 C ₁₅ H ₁₀ O ₃ N (-NH ₃) [92]	196.0751 C ₁₃ H ₁₀ ON (-C ₂ O ₂) [100] 208.0751 C ₁₄ H ₁₀ ON (-CO ₂) [43] 224.0737 C ₁₄ H ₁₀ O ₂ N (-CO) [43]		
		196.0752 C ₁₃ H ₁₀ ON (-C ₂ H ₃ O ₂ N) [6.6]	-		
	B 12.67	252.0655 C ₁₅ H ₁₀ O ₃ N (-NH ₃) [100]	196.0751 C ₁₃ H ₁₀ ON (-C ₂ O ₂) [100] 208.0751 C ₁₄ H ₁₀ ON (-CO ₂) [43] 224.0701 C ₁₄ H ₁₀ O ₂ N (-CO) [42]		[1]
		226.0861 C ₁₄ H ₁₂ O ₂ N (-CHON) [96.4]	198.0906 C ₁₃ H ₁₂ ON (-CO) [100] 196.0751 C ₁₃ H ₁₀ ON (-CH ₂ O) [4.5]		
		196.0752 C ₁₃ H ₁₀ ON (-C ₂ H ₃ O ₂ N) [8.5]	-		
	C 13.13	226.0860 C ₁₄ H ₁₂ O ₂ N (-CHON) [100]	198.0907 C ₁₃ H ₁₂ ON (-CO) [100] 208.0750 C ₁₄ H ₁₀ ON (-H ₂ O) [28]		[1]
		224.0706 C ₁₄ H ₁₂ O ₂ N (-CH ₃ ON) [21.7]	-		

		252.0653 C ₁₅ H ₁₀ O ₃ N (-NH ₃) [15.7]	224.0699 C ₁₄ H ₁₀ O ₂ N (-CO) [100]		
D 14.07		226.0859 C ₁₄ H ₁₂ O ₂ N (-CHON) [100]	180.0801 C ₁₃ H ₁₀ N (-CH ₂ O ₂) [100] 198.0906 C ₁₃ H ₁₂ ON (-CO) [36]		[1]
E 15.02		251.0815 C ₁₅ H ₁₁ O ₂ N ₂ (-H ₂ O) [100]	180.0800 C ₁₃ H ₁₀ N(C ₂ HO ₂ N)[100] 208.0749 C ₁₄ H ₁₀ ON (-CHON)[85] 223.0859 C ₁₄ H ₁₁ ON ₂ (-CO)[18.5]		[1]
		226.0860 C ₁₄ H ₁₂ O ₂ N (-CHON) [34.3]	-		
		224.0705 C ₁₄ H ₁₀ O ₂ N (-CH ₃ ON) [22.1]	-		
		252.0654 C ₁₅ H ₁₀ O ₃ N (-NH ₃) [21.8]	-		
F 15.55		226.0859 C ₁₄ H ₁₂ O ₂ N (-CHON) [100]	198.0906 C ₁₃ H ₁₂ ON (-CO) [100] 208.0749 C ₁₄ H ₁₀ ON (-H ₂ O) [76.4]		[1]
		224.0704 C ₁₄ H ₁₀ O ₂ N (-CH ₃ ON)[18.6]	-		
		252.0653 C ₁₅ H ₁₀ O ₃ N (-NH ₃) [6.5]	-		
G 16.37		251.0814 C ₁₅ H ₁₁ O ₂ N ₂ (-H ₂ O) [100]	208.0751 C ₁₄ H ₁₀ ON (-CHON) [100] 223.0859 C ₁₄ H ₁₁ ON ₂ (-CO) [18.5] 180.0801 C ₁₃ H ₁₀ N(C ₂ HO ₂ N) [10]		[1]
		226.0860 C ₁₄ H ₁₂ O ₂ N (-CHON) [26]	208.0750 C ₁₄ H ₁₀ ON (-H ₂ O) [100] 198.0906 C ₁₃ H ₁₂ ON (-CO) [45.2] 180.0800 C ₁₃ H ₁₀ N(C ₂ HO ₂ N) [27]		
H 16.50		251.0815 C ₁₅ H ₁₁ O ₂ N ₂ (-H ₂ O) [100]	208.0751 C ₁₄ H ₁₀ ON (-CHON) [100] 223.0861 C ₁₄ H ₁₁ ON ₂ (-CO) [13.8] 180.0802 C ₁₃ H ₁₀ N(C ₂ HO ₂ N) [8.2]		[1]
		208.0755 C ₁₄ H ₁₀ ON (-CH ₃ O ₂ N) [54.6]	-		
		223.0865 C ₁₄ H ₁₁ ON ₂ (-CH ₂ O ₂) [31]	-		
		226.0861 C ₁₄ H ₁₂ O ₂ N (-CHON) [21]	-		
		180.0804 C ₁₃ H ₁₀ N (-C ₂ H ₃ O ₃ N) [15]	-		
267.0769 C₁₅H₁₁O₃N₂⁺	A 12.85	249.0693 C ₁₅ H ₉ O ₂ N ₂ (-H ₂ O) [100] 224.0737 C ₁₄ H ₁₀ O ₂ N (-CHON) [63.5] 196.0782 C ₁₃ H ₁₀ ON (-C ₂ HO ₂ N) [58]	221.0706 C ₁₄ H ₉ ON ₂ (-CO) [100]		[1]
	B 14.63	224.0736 C ₁₄ H ₁₀ O ₂ N (-CHON) [100] 196.0781 C ₁₃ H ₁₀ ON (-C ₂ HO ₂ N) [82] 239.0847 C ₁₄ H ₁₁ O ₂ N (-CO) [18]	- - -		[1]
	C 15.48	224.0736 C ₁₄ H ₁₀ O ₂ N (-CHON) [100] 196.0782 C ₁₃ H ₁₀ ON (-C ₂ HO ₂ N) [42] 239.0847 C ₁₄ H ₁₁ O ₂ N (-CO) [9]	180.0801 C ₁₃ H ₁₀ N (-CO ₂) [100] 196.0751 C ₁₃ H ₁₀ ON (-CO) [60] 168.0800 C ₁₂ H ₁₀ N (-CO) [20] 168.0799 C ₁₂ H ₁₀ N (-CO) [100] -		[1]
	D 17.49	224.0738 C ₁₄ H ₁₀ O ₂ N (-CHON) [100] 196.0784 C ₁₃ H ₁₀ ON (-C ₂ HO ₂ N) [48] 250.0535 C ₁₅ H ₈ O ₃ N ₂ (-NH ₃) [54] 239.0851 C ₁₄ H ₁₁ O ₂ N (-CO) [6]	196.0750 C ₁₃ H ₁₀ ON (-CO) [100] - 194.0596 C ₁₃ H ₈ ON (-C ₂ HON) [100] 222.0545 C ₁₄ H ₈ O ₂ (-CO) [50] -		[1]

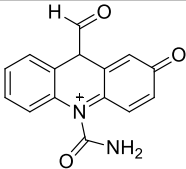
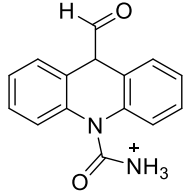
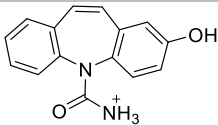
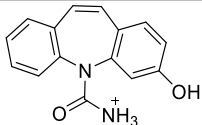
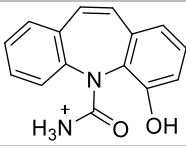
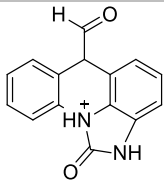
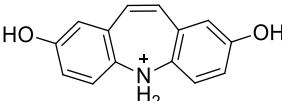
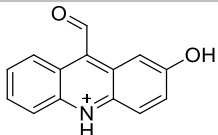
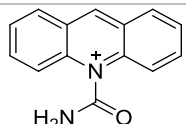
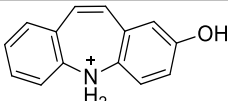
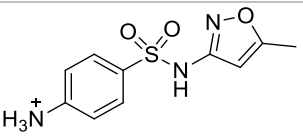
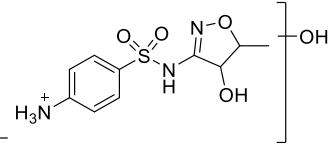
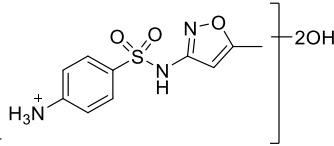
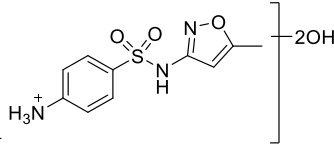
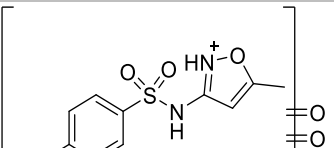
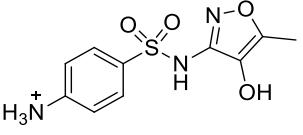
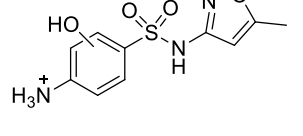
	E 18.03	196.0781 C ₁₃ H ₁₀ ON (-C ₂ HO ₂ N) [100]	-		[1]
		224.0735 C ₁₄ H ₁₀ O ₂ N (-CHON) [65]	168.0800 C ₁₂ H ₁₀ N (-CO) [100]		
		239.0847 C ₁₄ H ₁₁ O ₂ N (-CO) [15]	196.0781 C ₁₃ H ₁₀ ON (-CO) [100]		
253.0976 C ₁₅ H ₁₃ N ₂ O ₂ ⁺	A 14.24	236.0706 C ₁₅ H ₁₀ O ₂ N (-NH ₃) [100]	-		[1]
		210.0943 C ₁₄ H ₁₂ ON (-CHON) [58]	182.0957 C ₁₃ H ₁₂ N (-CO) [100] 180.0800 C ₁₃ H ₁₀ N (-CH ₂ O)		
		180.0832 C ₁₃ H ₁₀ N (-C ₂ H ₃ O ₂ N) [11.5]	-		
	B 16.69	210.0911 C ₁₄ H ₁₂ ON (-CHON) [100]	182.0957 C ₁₃ H ₁₂ N (-CO) [100] 192.0799 C ₁₄ H ₁₀ N (-H ₂ O) [25]		[1]
		208.0757 C ₁₄ H ₁₀ ON (-CH ₃ ON) [19]	180.0800 C ₁₃ H ₁₀ N (-CH ₂ O) [100]		
		236.0705 C ₁₅ H ₁₀ O ₂ N [16]	208.0751 C ₁₄ H ₁₀ ON (-CO) [100]		
	C 17.80	210.0910 C ₁₄ H ₁₂ ON (-CHON) [100]	182.0958 C ₁₃ H ₁₂ N (-CO) [100] 192.0799 C ₁₄ H ₁₀ N (-H ₂ O) [8.5]		[1]
		208.0757 C ₁₄ H ₁₀ ON (-CH ₃ ON) [12]	180.0800 C ₁₃ H ₁₀ N (-CH ₂ O) [100]		
		236.0705 C ₁₅ H ₁₀ O ₂ N [6]	208.0751 C ₁₄ H ₁₀ ON (-CO) [100]		
	D 18.55	210.0910 C ₁₄ H ₁₂ ON (-CHON) [100]	182.0956 C ₁₃ H ₁₂ N (-CO) [100] 192.0799 C ₁₄ H ₁₀ N (-H ₂ O) [45]		[1]
251.0820 C ₁₅ H ₁₁ O ₂ N ₂ ⁺	16.37	180.0805 C ₁₃ H ₁₀ N (-C ₂ HO ₂ N) [100]	-		[1]
		208.0756 C ₁₄ H ₁₀ ON (-CHON) [84]	180.0801 C ₁₃ H ₁₀ N (-CO) [100]		
		223.0865 C ₁₄ H ₁₁ ON ₂ (-CO) [17.6]	-		
226.0867 C ₁₄ H ₁₂ O ₂ N ⁺	28.59	208.0705 C ₁₄ H ₁₀ ON ⁺ (-H ₂ O) [100]	-		This work
		180.0761 C ₁₃ H ₁₀ N ⁺ (-CH ₂ O ₂)	-		
		198.0863 C ₁₃ H ₁₂ ON ⁺ (-CO)	-		
224.0710 C ₁₄ H ₁₀ O ₂ N ⁺	22.03	222.0555 C ₁₄ H ₈ NO ₂ (-H ₂) [100]	-		[2]
		178.0657 C ₁₃ H ₈ N (-CH ₂ O ₂) [40]	-		
		206.0605 C ₁₄ H ₈ NO (-H ₂ O) [30]	-		
		196.0762 C ₁₃ H ₁₀ NO (-CO) [10]	-		
223.0869 C ₁₄ H ₁₁ ON ₂ ⁺	14.99	180.0761 C ₁₃ H ₁₀ N ⁺ (-CHON)	-		This work
210.0918 C ₁₄ H ₁₂ NO	10.82	-	-		This work

Table S10. Sulfamethoxazole

Precursor ion [M+H] ⁺	t _R (min)	Product ions		Structure	Ref.
		MS ²	MS ³		
SMX 254.0598 C₁₀H₁₂O₃N₃S⁺	15.24	156.0111 C ₆ H ₆ NO ₂ S ⁺ (-C ₄ H ₆ ON ₂) [98]	108.0438 C ₆ H ₆ ON ⁺ (-SO) [100] 92.0488 C ₆ H ₆ N (-SO ₂) [27]		[3, 4,5]
		188.0819 C ₁₀ H ₁₀ ON ₃ ⁺ (-H ₂ O ₂ S) [100]	160.0869 C ₉ H ₁₀ N ₃ (-CO) [100]		
		108.0439 C ₆ H ₆ ON ⁺ (-C ₄ H ₆ O ₂ N ₂ S) [21.50]	-		
		99.0547 C ₄ H ₇ ON ₂ ⁺ (-C ₆ H ₅ O ₂ NS) [1]			
		94.06453 C ₆ H ₈ N ⁺ (-C ₄ H ₄ O ₃ N ₂ S) [3]	-		
		92.0488 C ₆ H ₆ N ⁺ (-C ₄ H ₆ O ₃ N ₂ S) [10]	-		
288.0654 C₁₀H₁₄O₅N₃S⁺	6.77	270.0475 C ₁₀ H ₁₂ O ₄ N ₃ S ⁺ (-H ₂ O) [100]			[3,5]
		206.08717 C ₁₀ H ₁₂ O ₂ N ₃ ⁺ (-H ₂ O ₃ S) [9.30]			
		160.0869 C ₉ H ₁₀ N ₃ ⁺ (-CH ₄ O ₅ S) [8.97]			
		188.08188 C ₁₀ H ₁₀ ON ₃ (-H ₄ O ₄ S) [15.50]			
286.0497 C₁₀H₁₂O₅N₃S⁺	A 9.98	156.0111 C ₆ H ₆ NO ₂ S ⁺ (-C ₄ H ₆ N ₂ O ₂) [5]			<i>This work</i>
		108.0439 C ₆ H ₆ ON ⁺ (-C ₄ H ₆ O ₄ N ₂ S) [4.80]			
		220.0660 C ₁₀ H ₁₀ N ₃ O ₃ ⁺ (-H ₂ O ₂ S) [8]			
		177.0629 C ₉ H ₉ N ₂ O ₂ ⁺ (-CH ₃ NO ₃ S) [100]			
	B 12.08	269.0397 C ₁₀ H ₁₁ O ₄ N ₃ S ⁺ (-HO·) [100]			<i>This work</i>
		176.0771 C ₉ H ₁₀ N ₃ O ⁺ (-CH ₂ O ₄ S) [70]			
		268.0318 C ₁₀ H ₁₀ O ₄ N ₃ S ⁺ (-H ₂ O) [64]			
		156.0111 C ₆ H ₆ NO ₂ S ⁺ (-C ₄ H ₆ N ₂ O ₂) [26]			
		108.0439 C ₆ H ₆ ON ⁺ (-C ₄ H ₆ O ₄ N ₂ S) [5.08]			
		220.0660 C ₁₀ H ₁₀ N ₃ O ₃ ⁺ (-H ₂ O ₂ S) [26.3]			
	23.42	-			<i>This work</i>
270.0548 C₁₀H₁₂O₄N₃S⁺	A 10.67	156.0111 C ₆ H ₆ NO ₂ S ⁺ (-C ₄ H ₆ ON ₂) [84]			[4]
		160.0869 C ₉ H ₁₀ N ₃ ⁺ (-CH ₂ O ₄ S) [97]			
		204.0717 C ₁₀ H ₁₀ N ₃ O ₂ ⁺ (-H ₂ O ₂ S) [100]			
	B 14.98	108.0439 C ₆ H ₆ ON ⁺ (-C ₄ H ₆ O ₄ N ₂ S) [89]			[3, 5]
		124.0358 C ₆ H ₆ NO ₂ ⁺ (-C ₄ H ₆ N ₂ O ₂ S) [13]			
		189.0611 C ₆ H ₉ N ₂ O ₃ S ⁺ (-H ₃ O ₂ NS) [33.40]			

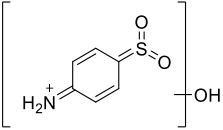
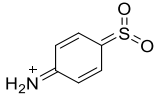
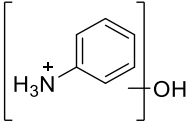
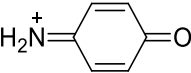
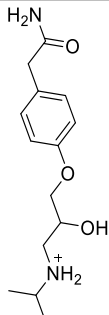
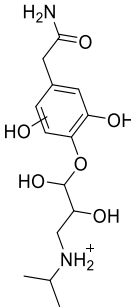
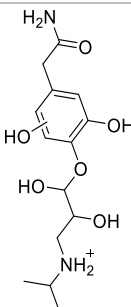
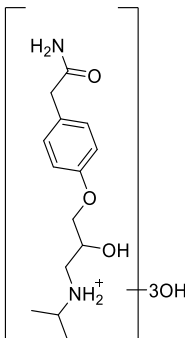
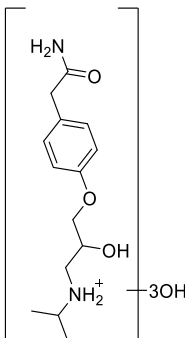
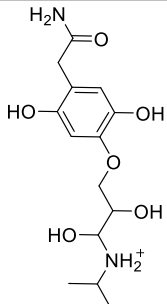
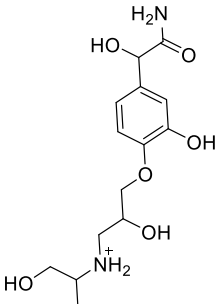
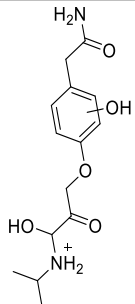
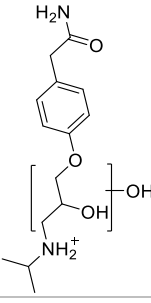
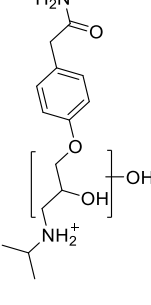
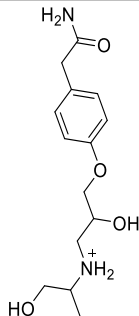
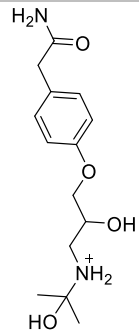
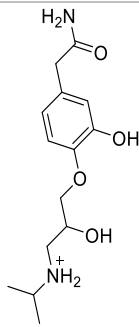
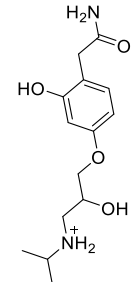
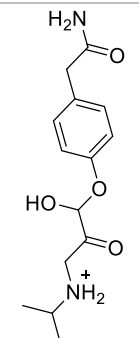
		204.0717 C ₁₀ H ₁₀ N ₃ O ₂ ⁺ (-H ₂ O ₂ S) [55]			
		99.0522 C ₄ H ₇ N ₂ O ⁺ (-C ₆ H ₅ O ₃ NS) [100]			
		172.0018 C ₆ H ₆ NO ₃ S ⁺ (-C ₄ H ₆ N ₂ O) [39]			
172.0060 C₆H₆O₃NS⁺	14.94	-			<i>This work</i>
156.0111 C₆H₆O₂NS⁺	15.20				[3]
110.0597 C₆H₈ON⁺	1.67	-			<i>This work</i>
108.0440 C₆H₆ON⁺	14.97	-			[3]

Table S11. Atenolol

Precursor ion [M+H] ⁺	t _R min	Product ions		Structure	Ref.
		MS ²	MS ³		
ATL 267.1708 C ₁₄ H ₂₃ N ₂ O ₃ ⁺	4.96	190.0868 C ₁₁ H ₁₂ NO ₂ ⁺ (-C ₃ H ₁₁ NO) [100]	145.0652 C ₁₀ H ₉ O (-CH ₃ NO) [100] 173.0602 C ₁₁ H ₉ O ₂ (-NH ₃) [20]		[6]
		225.1239 C ₁₁ H ₁₇ N ₂ O ₃ ⁺ (-C ₃ H ₆) [90.19]	-		
		208.0973 C ₁₁ H ₁₄ NO ₃ ⁺ (-C ₃ H ₉ N) [37.25]	-		
		250.1443 C ₁₄ H ₂₀ NO ₃ ⁺ (-NH ₃) [9.80]	190.0868 C ₁₁ H ₁₂ O ₂ N (-C ₃ H ₈ O) [18] 173.0602 C ₁₁ H ₉ O ₂ (-C ₃ H ₁₁ NO) [100]		
		116.1059 C ₆ H ₁₄ NO ⁺ (-C ₈ H ₉ NO ₂) [15.68]	74.0589 C ₃ H ₈ ON (-C ₃ H ₆) [100] 56.0488 C ₃ H ₆ N (-C ₃ H ₈ O) [20]		
315.1558 C ₁₄ H ₂₃ N ₂ O ₆ ⁺	A 1.70	298.1263 C ₁₄ H ₂₀ O ₆ N ⁺ (-NH ₃) [100]	116.1059 C ₆ H ₁₄ NO ⁺ (-C ₈ H ₆ O ₅) [100] 256.1176 C ₁₂ H ₁₈ O ₅ N ⁺ (-C ₂ H ₂ O) [85] 184.0961 C ₉ H ₁₄ O ₃ N ⁺ (-C ₅ H ₇ O ₃ N) [55] 254.1383 C ₁₃ H ₂₀ O ₄ N ⁺ (-CO ₂) [35] 280.1178 C ₁₄ H ₁₈ O ₅ N ⁺ (-H ₂ O) [20]		[6]
	B 2.24	298.1263 C ₁₄ H ₂₀ O ₆ N ⁺ (-NH ₃) [100]	116.1059 C ₆ H ₁₄ NO ⁺ (-C ₈ H ₆ O ₅) [100] 256.1176 C ₁₂ H ₁₈ O ₅ N ⁺ (-C ₂ H ₂ O) [85] 184.0961 C ₉ H ₁₄ O ₃ N ⁺ (-C ₅ H ₇ O ₃ N) [55] 254.1383 C ₁₃ H ₂₀ O ₄ N ⁺ (-CO ₂) [35] 280.1178 C ₁₄ H ₁₈ O ₅ N ⁺ (-H ₂ O) [20]		[6]
	C 2.93	297.1422 C ₁₄ H ₂₁ O ₅ N ₂ ⁺ (-H ₂ O) [100]	134.1165 C ₆ H ₁₆ O ₂ N ⁺ (-C ₈ H ₅ O ₃ N) [100]		[6]
		271.1631 C ₁₀ H ₂₅ O ₇ N ⁺ (-C ₄ H ₂ ON) [40]	-		
		116.1059 C ₆ H ₁₄ NO ⁺ (-C ₈ H ₉ NO ₅) [20]	-		
	D 4.62	297.1422 C ₁₄ H ₂₁ O ₅ N ₂ ⁺ (-H ₂ O) [100]	134.1165 C ₆ H ₁₆ O ₂ N ⁺ (-C ₈ H ₅ O ₃ N) [100]		[6]
		254.1383 C ₁₃ H ₂₀ O ₄ N ⁺ (-CH ₃ O ₂ N) [20]	236.0558 C ₁₁ H ₁₀ O ₅ N ⁺ (-C ₂ H ₁₀ O) [100]		
		298.1263 C ₁₄ H ₂₀ O ₆ N ⁺ (-NH ₃) [70]	134.1165 C ₆ H ₁₆ O ₂ N ⁺ (-C ₈ H ₄ O ₄) [100]		
		134.1165 C ₆ H ₁₆ O ₂ N ⁺ (-C ₈ H ₇ O ₄ N) [20]	-		
		116.1059 C ₆ H ₁₄ NO ⁺ (-C ₈ H ₉ NO ₅) [20]	-		

	E 4.92	298.1263 C ₁₄ H ₂₀ O ₆ N ⁺ (-NH ₃) [100]	134.1165 C ₆ H ₁₆ O ₂ N ⁺ (-C ₈ H ₄ O ₄) [100] 280.1179 C ₁₄ H ₁₈ O ₅ N ⁺ (-H ₂ O) [15] 116.1059 C ₆ H ₁₄ NO ⁺ (-C ₈ H ₆ O ₅) [10]		[6]
		134.1165 C ₆ H ₁₆ O ₂ N ⁺ (-C ₈ H ₇ O ₄ N) [50]	116.1055 C ₆ H ₁₄ NO ⁺ (-H ₂ O) [100] 92.0692 C ₃ H ₁₀ O ₂ N ⁺ (-C ₃ H ₆) [50] 72.0796 C ₄ H ₁₀ N (-C ₂ H ₆ O ₂) [30] 74.0589 C ₃ H ₈ ON (-C ₃ H ₈ O) [25]		
	F 5.48	297.1422 C ₁₄ H ₂₁ O ₅ N ₂ ⁺ (-H ₂ O) [100]	280.1178 C ₁₄ H ₁₈ O ₅ N ⁺ (-NH ₃) [100] 239.1033 C ₁₁ H ₁₅ O ₄ N ₂ ⁺ (-C ₃ H ₆ O) [40] 240.0873 C ₁₁ H ₁₄ O ₅ N ⁺ (-C ₃ H ₇ N) [38] 134.1171 C ₆ H ₁₆ O ₂ N ⁺ (-C ₈ H ₅ O ₃ N) [35] 279.1351 C ₁₄ H ₁₉ O ₄ N ₂ ⁺ (-H ₂ O) [25] 166.0497 C ₈ H ₈ O ₃ N ⁺ (-C ₆ H ₁₃ O ₂ N) [18]		[6]
		134.1165 C ₆ H ₁₆ O ₂ N ⁺ (-C ₈ H ₇ O ₄ N) [15]	116.1055 C ₆ H ₁₄ NO ⁺ (-H ₂ O) [100] 92.0692 C ₃ H ₁₀ O ₂ N ⁺ (-C ₃ H ₆) [45]		
297.1450 C ₁₄ H ₂₁ N ₂ O ₅ ⁺	8.03	280.1160 C ₁₄ H ₁₈ O ₅ N ⁺ (-NH ₃) [100]	262.1078 C ₁₄ H ₁₆ O ₄ N ⁺ (-H ₂ O) [100] 116.1067 C ₆ H ₁₄ NO ⁺ (-C ₈ H ₄ O ₄) [93] 221.0448 C ₁₁ H ₉ O ₅ ⁺ (-C ₃ H ₉ N) [67] 238.0716 C ₁₁ H ₁₂ O ₅ N ⁺ (-C ₃ H ₆) [7]		[6]
		238.0693 C ₁₁ H ₁₂ O ₅ N ⁺ (-C ₃ H ₉) [22]	-		
		116.1067 C ₆ H ₁₄ NO ⁺ (-C ₈ H ₇ O ₄ N) [9]	-		
283.1658 C ₁₄ H ₂₃ O ₄ N ₂ ⁺	A 2.32	265.2523 C ₁₄ H ₂₁ O ₃ N ₂ ⁺ (-H ₂ O) [55]	223.1072 C ₁₁ H ₁₅ O ₃ N ₂ ⁺ (-C ₃ H ₆) [100] 206.0805 C ₁₁ H ₁₂ O ₃ N ⁺ (-C ₃ H ₉ N) [45]		[6]
		225.1239 C ₁₁ H ₁₇ N ₂ O ₃ ⁺ (-C ₃ H ₆ O) [55]	-		
		224.1275 C ₁₂ H ₁₈ O ₃ N ⁺ (-C ₂ H ₅ ON) [35]	-		
		223.1083 C ₁₁ H ₁₅ O ₃ N ₂ ⁺ (-C ₃ H ₉ O) [40]	164.0711 C ₉ H ₁₀ O ₂ N ⁺ (-C ₂ H ₅ ON) [100]		
		116.1059 C ₆ H ₁₄ ON ⁺ (-C ₈ H ₉ O ₃ N) [100]	72.0796 C ₄ H ₁₀ N (-C ₂ H ₄ O) [100]		
		164.0711 C ₉ H ₁₀ O ₂ N ⁺ (-C ₅ H ₁₃ O ₂ N) [40]	122.0586 C ₇ H ₈ ON (-C ₂ H ₂ O) [100]		
	B 2.93	225.1239 C ₁₁ H ₁₇ N ₂ O ₃ ⁺ (-C ₃ H ₆ O) [55]	-		[6]
		223.1083 C ₁₁ H ₁₅ O ₃ N ₂ ⁺ (-C ₃ H ₉ O) [40]	164.0711 C ₉ H ₁₀ O ₂ N ⁺ (-C ₂ H ₅ ON) [100]		
		265.2523 C ₁₄ H ₂₁ O ₃ N ₂ ⁺ (-H ₂ O) [55]	223.1072 C ₁₁ H ₁₅ O ₃ N ₂ ⁺ (-C ₃ H ₆) [100] 206.0805 C ₁₁ H ₁₂ O ₃ N ⁺ (-C ₃ H ₉ N) [45]		
		224.1275 C ₁₂ H ₁₈ O ₃ N ⁺ (-C ₂ H ₅ ON) [35]	-		
		164.0711 C ₉ H ₁₀ O ₂ N ⁺ (-C ₅ H ₁₃ O ₂ N) [40]	122.0586 C ₇ H ₈ ON (-C ₂ H ₂ O) [100]		
		116.1059 C ₆ H ₁₄ ON ⁺ (-C ₈ H ₉ O ₃ N) [100]	72.0796 C ₄ H ₁₀ N (-C ₂ H ₄ O) [100]		
	C 4.17	116.1059 C ₆ H ₁₄ ON ⁺ (-C ₈ H ₉ O ₃ N) [100]	72.0796 C ₄ H ₁₀ N (-C ₂ H ₄ O) [100] 74.0589 C ₃ H ₈ ON (-C ₃ H ₆) [20]		[6]

		265.2523 C ₁₄ H ₂₁ O ₃ N ₂ ⁺ (-H ₂ O) [10]	248.1277 C ₁₄ H ₁₈ O ₃ N (-NH ₃) [100] 116.1059 C ₆ H ₁₄ NO ⁺ (-C ₆ H ₇ NO ₂) [25]		
D 4.85		190.0868 C ₁₁ H ₁₂ O ₂ N ⁺ (-C ₃ H ₁₁ O ₂ N) [8]	-		[6]
		265.1552 C ₁₄ H ₂₁ O ₃ N ₂ ⁺ (-H ₂ O) [100]	190.0855 C ₁₁ H ₁₂ O ₂ N ⁺ (-C ₃ H ₉ ON) [100] 248.1277 C ₁₄ H ₁₈ O ₃ N ⁺ (-NH ₃) [55] 114.0902 C ₆ H ₁₂ ON (-C ₈ H ₉ O ₂ N) [40] 145.0638 C ₁₀ H ₉ O (-C ₄ H ₁₂ N ₂ O ₂) [20] 220.1326 C ₁₃ H ₁₈ O ₂ N (-CH ₃ ON) [20]		
		191.0708 C ₁₁ H ₁₁ O ₃ ⁺ (-C ₃ H ₁₂ ON ₂) [10]	-		
E 5.34		241.1188 C ₁₁ H ₁₇ O ₄ N ₂ ⁺ (-C ₃ H ₆) [100]	224.0921 C ₁₁ H ₁₄ O ₄ N ⁺ (-NH ₃) [100] 178.0863 C ₁₀ H ₁₂ O ₂ N ⁺ (-CH ₅ O ₂ N) [20] 74.0594 C ₃ H ₈ ON ⁺ (-C ₈ H ₉ O ₃ N) [15]		[6]
		206.0817 C ₁₁ H ₁₂ O ₃ N ⁺ (-C ₃ H ₁₁ ON) [95]	178.0863 C ₁₀ H ₁₂ O ₂ N ⁺ (-CO) [100] 161.0597 C ₁₀ H ₉ O ₂ ⁺ (-CH ₃ ON) [70] 189.0548 C ₁₁ H ₉ O ₃ (-NH ₃) [65]		
		266.1392 C ₁₄ H ₂₀ O ₄ N ⁺ (-NH ₃) [20]	206.0795 C ₁₁ H ₁₂ O ₃ N ⁺ (-C ₃ H ₈ O) [100] 248.1262 C ₁₄ H ₁₈ O ₃ N ⁺ (-H ₂ O) [30] 178.0847 C ₁₀ H ₁₂ O ₂ N ⁺ (-C ₄ H ₈ O ₂) [20] 189.0530 C ₁₁ H ₉ O ₃ ⁺ (-C ₃ H ₁₁ ON) [15]		
		189.0552 C ₁₁ H ₉ O ₃ (-C ₃ H ₁₂ ON ₂) [20]	161.0597 C ₁₀ H ₉ O ₂ ⁺ (-CO) [100] 133.0646 C ₉ H ₉ O (-C ₂ O ₂) [25]		
		178.0854 C ₁₀ H ₁₂ O ₂ N (-C ₄ H ₁₁ O ₂ N) [50]	-		
		224.0922 C ₁₁ H ₁₄ O ₄ N (-C ₃ H ₉ N) [50]	206.0817 C ₁₁ H ₁₂ O ₃ N ⁺ (-H ₂ O) [100] 178.0847 C ₁₀ H ₁₂ O ₂ N ⁺ (-CH ₂ O ₂) [35]		
F 8.76		266.1392 C ₁₄ H ₂₀ O ₄ N ⁺ (-NH ₃) [100]	224.0922 C ₁₁ H ₁₄ O ₄ N ⁺ (-C ₃ H ₈) [95] 161.0602 C ₁₀ H ₉ O ₂ ⁺ (-C ₄ H ₁₁ O ₂ N) [25] 189.0552 C ₁₁ H ₉ O ₃ ⁺ (-C ₃ H ₁₁ ON) [100] 220.1315 C ₁₃ H ₁₈ O ₂ N ⁺ (-CH ₂ O ₂) [25] 116.1075 C ₆ H ₁₄ ON ⁺ (-C ₈ H ₆ O ₃) [25] 248.1262 C ₁₄ H ₁₈ O ₃ N ⁺ (-H ₂ O) [8]		[6]
		116.1075 C ₆ H ₁₄ ON ⁺ (-C ₈ H ₉ O ₃ N) [70]	72.0796 C ₄ H ₁₀ N ⁺ (-C ₂ H ₄ O) [100] 74.0589 C ₃ H ₈ ON ⁺ (-C ₃ H ₆) [65]		
		194.0817 C ₁₀ H ₁₂ O ₃ N (-C ₄ H ₁₁ ON) [25]	-		
281.1502 C₁₄H₂₁O₄N₂⁺	A 4.86	239.1031 C ₁₁ H ₁₅ O ₄ N ₂ ⁺ (-C ₃ H ₆) [100]	-		[6]
		263.1396 C ₁₄ H ₁₉ O ₃ N ₂ ⁺ (-H ₂ O) [70]	-		
		166.0499 C ₈ H ₈ O ₃ N ⁺ (-C ₆ H ₁₃ ON) [45]	-		
		221.0924 C ₁₁ H ₁₃ O ₃ N ₂ ⁺ (-C ₃ H ₈ O) [25]	-		
		114.0911 C ₆ H ₁₂ ON ⁺ (-C ₈ H ₉ O ₃ N) [20]	-		
	B 5.69	263.1395 C ₁₄ H ₁₉ O ₃ N ₂ ⁺ (-H ₂ O) [9]	204.0660 C ₁₁ H ₁₀ O ₃ N ⁺ (-C ₃ H ₉ N) [15] 218.1178 C ₁₃ H ₁₆ O ₂ N ⁺ (-CH ₃ O) [100]		[6]

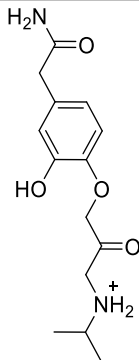
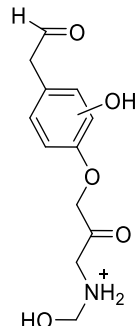
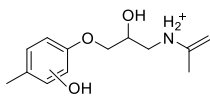
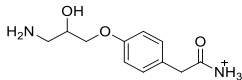
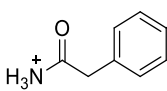
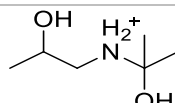
		239.1030 C ₁₁ H ₁₅ O ₄ N ₂ ⁺ (-C ₃ H ₆) [17]	194.0804 C ₁₀ H ₁₂ O ₃ N ⁺ (-CH ₃ ON) [100] 121.0273 C ₇ H ₅ O ₂ ⁺ (-C ₄ H ₁₀ O ₂ N ₂) [80]		
		116.1067 C ₆ H ₁₄ ON ⁺ (-C ₈ H ₇ O ₃ N) [100]	74.0242 C ₃ H ₈ ON ⁺ (-C ₃ H ₆) [100]		
		218.1173 C ₁₃ H ₁₆ O ₂ N ⁺ (-CH ₅ O ₂ N) [35]	176.0707 C ₁₀ H ₁₀ O ₂ N ⁺ (-C ₃ H ₆) [100] 161.0597 C ₁₀ H ₉ O ₂ ⁺ (-C ₃ H ₇ N) [98]		
		194.0814 C ₁₀ H ₁₂ O ₃ N ⁺ (-C ₄ H ₉ ON) [34]	74.0242 C ₃ H ₈ ON ⁺ (-C ₃ H ₆) [15] 121.0281 C ₇ H ₅ O ₂ ⁺ (-C ₃ H ₇ ON) [100]		
		176.0707 C ₁₀ H ₁₀ O ₂ N ⁺ (-C ₄ H ₁₁ O ₂ N) [16]	121.0281 C ₇ H ₅ O ₂ ⁺ (-C ₃ H ₅ N) [100] 159.0441 C ₁₀ H ₇ O ₂ ⁺ (-NH ₃) [45]		
		204.0658 C ₁₁ H ₁₀ O ₃ N ⁺ (-C ₃ H ₁₁ ON) [7]	-		
		191.0701 C ₁₁ H ₁₁ O ₃ ⁺ (-C ₃ H ₁₁ ON) [70]	-		
		165.0546 C ₉ H ₉ O ₃ ⁺ (-C ₅ H ₁₃ ON) [33]	-		
		145.0647 C ₁₀ H ₉ O ⁺ (-C ₄ H ₁₃ O ₃ N) [100]	-		
254.1391 C₁₃H₂₀O₄N⁺	6.20	212.0920 C ₁₀ H ₁₄ O ₄ N ⁺ (-C ₃ H ₆) [100]	177.0547 C ₁₀ H ₉ O ₃ (-C ₃ H ₁₁ ON) [100] 133.0647 C ₉ H ₉ O (-CH ₅ O ₃ N) [21] 105.0695 C ₈ H ₉ ⁺ (-C ₂ H ₅ O ₄ N) [9] 194.0813 C ₁₀ H ₁₂ O ₃ N ⁺ (-H ₂ O) [6]		[6]
		177.0547 C ₁₀ H ₉ O ₃ (-C ₃ H ₁₁ ON) [84]	-		
		236.1287 C ₁₃ H ₁₈ NO ₃ ⁺ (-H ₂ O) [57]	177.0547 C ₁₀ H ₉ O ₃ (-C ₃ H ₉ N) [100] 194.0814 C ₁₀ H ₁₂ O ₃ N ⁺ (-C ₃ H ₆) (23) 98.0960 C ₆ H ₁₂ N ⁺ (-C ₇ H ₆ O ₃) [16]		
		194.0814 C ₁₀ H ₁₂ O ₃ N ⁺ (-C ₃ H ₈ O) [55]	-		
		105.0695 C ₈ H ₉ ⁺ (-C ₅ H ₁₁ O ₄ N) [10]	-		
238.1442 C₁₃H₂₀O₃N	7.09	220.1347 C ₁₃ H ₁₈ NO ₂ ⁺ (-H ₂ O) [7]	-		[7]
		196.0976 C ₁₀ H ₁₄ NO ₃ ⁺ (-C ₃ H ₆) [33]	-		
		178.0857 C ₁₀ H ₁₂ NO ₂ ⁺ (-C ₃ H ₈ O) [5]	-		
		161.0598 C ₁₀ H ₉ O ₂ ⁺ (-C ₃ H ₁₁ ON) [33]	-		
		149.0605 C ₉ H ₉ O ₂ ⁺ (-C ₄ H ₁₁ ON) [15]	-		
		133.0651 C ₉ H ₉ O ⁺ (-C ₄ H ₁₁ O ₂ N) [15]	-		
		123.0442 C ₇ H ₇ O ₂ ⁺ (-C ₆ H ₁₃ ON) [6]	-		
		267.1708 C ₁₄ H ₂₃ N ₂ O ₃ ⁺ [100]	-		
225.1238 C₁₁H₁₇N₂O₃⁺	2.87	208.1000 C ₁₁ H ₁₄ NO ₃ ⁺ (-NH ₃) [60]	-		[7, 8]
		190.0875 C ₁₁ H ₁₂ O ₂ N ⁺ (-H ₅ NO) [100]	-		
		178.0881 C ₁₀ H ₁₂ NO ₂ ⁺ (-CH ₅ NO) [40]	-		
		145.0660 C ₁₀ H ₉ O ⁺ (-CH ₈ N ₂ O ₂) [90]	-		
		133.0655 C ₉ H ₉ O ⁺ (-C ₂ H ₈ N ₂ O ₂) [15]	-		
152.0706 C₈H₁₀O₂N	6.80	107.0488 C ₇ H ₇ O ⁺ (-CH ₃ ON) [100]	-		[8]
134.1173 C₆H₁₆O₂N	1.64	92.0702 C ₃ H ₁₀ O ₂ N ⁺ (-C ₃ H ₆) [20]	-		[6]
		116.1067 C ₆ H ₁₄ NO ⁺ (-H ₂ O) [100]	72.0802 C ₄ H ₁₀ N ⁺ (-C ₂ H ₄ O) [29] 74.0595 C ₃ H ₈ ON ⁺ (-C ₃ H ₆) [20]		

Table S12. Bisphenol A

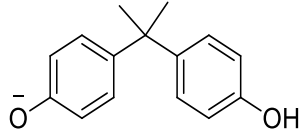
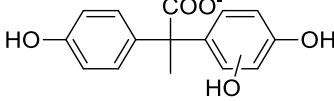
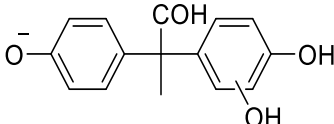
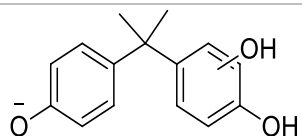
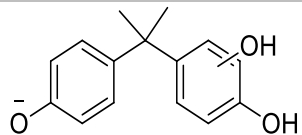
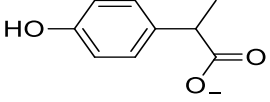
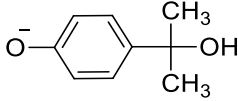
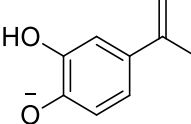
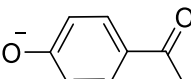
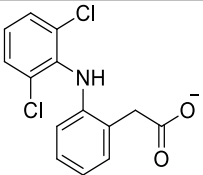
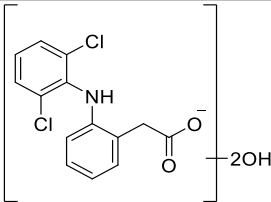
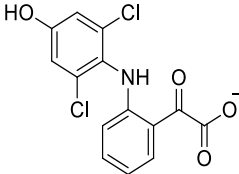
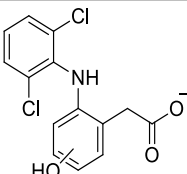
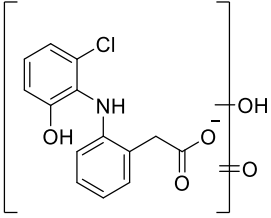
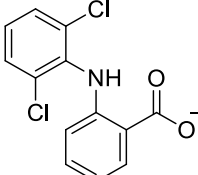
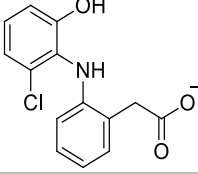
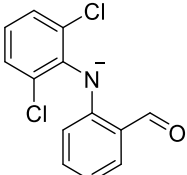
Precursor ion [M+H] ⁺	t _R (min)	Product ions	Structure	Ref.
		MS ²		
BPA 227.1105 C₁₅H₁₅O₂⁻	16.46	227.1105 C ₁₅ H ₁₅ O ₂ ⁻ [100] 133.0681 C ₉ H ₉ O (-C ₆ H ₆ O) [3] 212.0871 C ₁₄ H ₁₂ O ₂ ⁺ (-CH ₃) [50] ⁻		[9]
273.0796 C₁₅H₁₃O₅⁻	14.02	-		<i>This work</i>
257.0851 C₁₅H₁₃O₄⁻	17.67	229.0818 C ₁₄ H ₁₃ O ₃ ⁻ (-CO) [100] 163.0365 C ₉ H ₇ O ₃ ⁻ (-C ₆ H ₆ O) [12]		[9]
243.1057 C₁₅H₁₅O₃⁻	A 21.30	243.1057 C ₁₅ H ₁₅ O ₃ ⁻ [18.50] 93.0332 C ₆ H ₅ O ⁻ (-C ₉ H ₁₀ O ₂) [1] 149.0579 C ₉ H ₉ O ₂ ⁻ (-C ₆ H ₆ O) [3] 228.0824 C ₁₄ H ₁₂ O ₃ ⁺ (-CH ₃) [100]		[9]
		243.1057 C ₁₅ H ₁₅ O ₃ ⁻ [18.50] 228.0824 C ₁₄ H ₁₂ O ₃ ⁺ (-CH ₃) [100] 149.0579 C ₉ H ₉ O ₂ ⁻ (-C ₆ H ₆ O) [5.50]		
	B 24.39	243.1057 C ₁₅ H ₁₅ O ₃ ⁻ [18.50] 228.0824 C ₁₄ H ₁₂ O ₃ ⁺ (-CH ₃) [100] 149.0579 C ₉ H ₉ O ₂ ⁻ (-C ₆ H ₆ O) [5.50]		[9]
165.0432 C₉H₉O₃⁻	11.03	-		<i>This work</i>
151.0787 C₉H₁₁O₂	9.4	-		[10]
149.0605 C₉H₉O₂⁻	12.59	-		[9]
135.0472 C₈H₇O₂	10.21	93.0442 C ₆ H ₅ O ⁻ (-C ₂ H ₂ O) [100]		[9]

Table S13. Diclofenac

Precursor ion [M+H] ⁺	t _R (min)	Product ions		Structure	Ref.
		MS ²	MS ³		
DCF 294.0133 C₁₄H₁₀Cl₂NO₂⁺	25.67	250.0229 C ₁₃ H ₁₀ NCl ₂ (-CO ₂) [100]	214.0390 C ₁₃ H ₉ NCl (-HCl) [100]		[11]
325.9849 C₁₄H₁₀Cl₂NO₄	24.53	-	-		[11,12]
323.9878 C₁₄H₈Cl₂NO₄	24.73	279.9888 C ₁₃ H ₉ Cl ₂ NO ₂ ⁺ (-CO ₂) [100]			This work
		244.0127 (-CH ₂ O ₂ Cl) [15]			
310.0080 C₁₄H₁₀Cl₂NO₃	A 17.82	-			[11, 12]
	B 21.03	266.0097 C ₁₃ H ₁₀ Cl ₂ NO ⁺ (-CO ₂) [100] 230.0336 C ₁₃ H ₉ ClNO ⁺ (-CHClO ₂) [63] 194.0579 C ₁₃ H ₈ NO ⁺ (-CH ₂ O ₂ Cl ₂) [13]			
	C 21.70	-			
306.0217 C₁₄H₉ClNO₅	A 8.42	-			This work
	B 11.39	270.0358 C ₁₄ H ₈ NO ₅ ⁺ (-HCl) [100] 226.0468 C ₁₃ H ₈ NO ₃ ⁺ (-CH ₂ O ₂ Cl) [33]			
279.9972 C₁₃H₈Cl₂NO₂	11.36	-			This work
276.0469 C₁₄H₁₁ClNO₃	21.28	258.0282 C ₁₄ H ₉ ClNO ₂ ⁺ (-H ₂ O) [100]			This work
		232.0493 C ₁₃ H ₁₁ ClNO ⁺ (-CO ₂) [10]			
264.0024 C₁₃H₈Cl₂NO	19.30	228.0180 C ₁₃ H ₇ ClNO (-HCl) [100]			This work

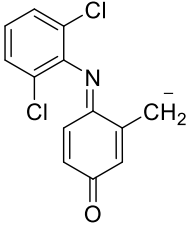
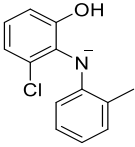
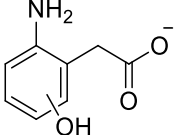
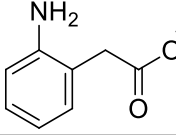
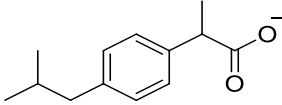
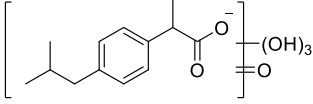
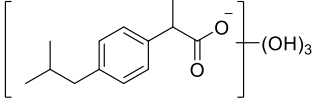
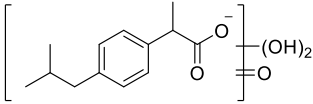
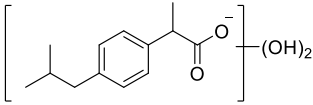
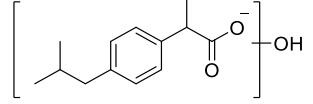
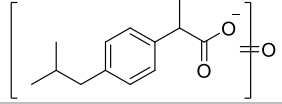
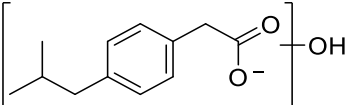
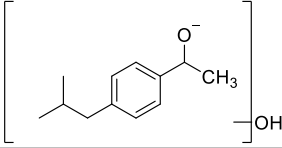
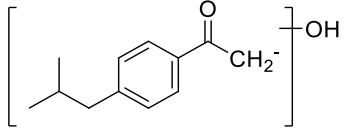
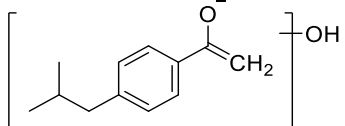
				
232.0563 C₁₃H₁₁ClNO	9.65	-		<i>This work</i>
166.0504 C₈H₈NO₃	A 11.20	-		[11]
	B 11.40	-		
150.0584 C₈H₈NO₂	5.04	-		[11]

Table S14. Ibuprofen

Precursor ion [M+H] ⁺	t _R (min)	Product ions		Structure	Ref.
		MS ²	MS ³		
IBP 205.1223 C₁₃H₁₇O₂⁻	28.12	161.1361 C ₁₂ H ₁₇ ⁻ (-CO ₂) [100]	-		[12, 13, 14]
		159.12054 C ₁₂ H ₁₅ ⁻ (-H ₂ CO ₂) [1]	-		
267.1270 C₁₄H₁₉O₅⁻	A 17.31	221.1140 C ₁₃ H ₁₇ O ₃ ⁻ (-CH ₂ O ₂) [100]			This work
		177.1252 C ₁₂ H ₁₇ O ⁻ (-C ₂ H ₂ O ₄) [65]			
	B 22.96	221.1140 C ₁₃ H ₁₇ O ₃ ⁻ (-CH ₂ O ₂) [100]			
		177.1252 C ₁₂ H ₁₇ O ⁻ (-C ₂ H ₂ O ₄) [83]			
253.1116 C₁₃H₁₇O₅⁻	A 14.22	-			This work
	B 15.59	-			
	C 16.01	-			
	D 17.02	-			
251.0943 C₁₃H₁₅O₅⁻	A 16.60	-			This work
	B 17.70	-			
237.1161 C₁₃H₁₇O₄⁻	A 17.71	-			[13]
	B 18.61	-			
	C 19.28	-			
221.1209 C₁₃H₁₇O₃⁻	A 15.92	-			[12, 13]
	B 17.23	-			
	C 20.33	177.1252 C ₁₂ H ₁₇ O ⁻ (-CO ₂) [100]			
	D 22.70	177.1252 C ₁₂ H ₁₇ O ⁻ (-CO ₂) [55]			
		159.1150 C ₁₂ H ₁₅ ⁻ (-CH ₂ O ₃) [100]			
	E 23.33	177.1252 C ₁₂ H ₁₇ O ⁻ (-CO ₂) [100]			
219.0980 C₁₃H₁₅O₃⁻	A 18.88	-			This work
207.1055 C₁₂H₁₅O₃	28.19	191.0697 C ₁₁ H ₁₁ O ₃ ⁻ (-CH ₄)			[14]
		164.0500 C ₉ H ₈ O ₃ ⁻ (-C ₃ H ₇)			
		150.0306 C ₈ H ₆ O ₃ ⁻ (-C ₄ H ₉)			
		135.0453 C ₈ H ₇ O ₂ ⁻ (-C ₄ H ₈ O)			
		121.0293 C ₇ H ₅ O ₂ ⁻ (-C ₅ H ₁₀ O)			
		106.0453 C ₇ H ₆ O ⁻ (-C ₅ H ₉ O ₂)			
		93.0329 C ₆ H ₅ O ⁻ (-C ₆ H ₁₀ O ₂)			
193.12604 C₁₂H₁₇O₂⁻	A 16.47	177.0915 C ₁₁ H ₁₃ O ₂ ⁻ (-CH ₄)			[14]
		149.0966 C ₁₀ H ₁₃ O ⁻ (-C ₂ H ₄ O)			
	B 17.99	-			
191.1066 C₁₂H₁₅O₂⁻	A 10.91	177.0915 C ₁₁ H ₁₃ O ₂ ⁻ (-CH ₃)			[14]
		149.0966 C ₁₀ H ₁₃ O ⁻ (-C ₂ H ₂ O)			
		163.0759 C ₁₀ H ₁₁ O ₂ ⁻ (-C ₂ H ₄)			
		135.0809 C ₉ H ₁₁ O ⁻ (-C ₃ H ₄ O)			
	B 18.58	177.0915 C ₁₁ H ₁₃ O ₂ ⁻ (-CH ₃)			[14]
		149.0966 C ₁₀ H ₁₃ O ⁻ (-C ₂ H ₂ O)			
		163.0759 C ₁₀ H ₁₁ O ₂ ⁻ (-C ₂ H ₄)			

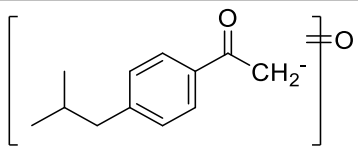
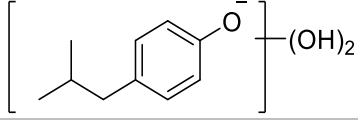
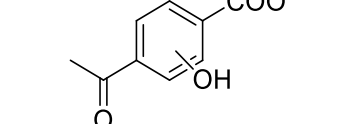
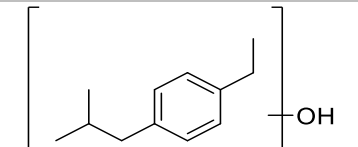
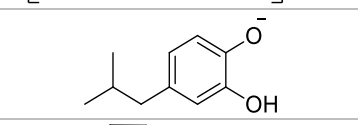
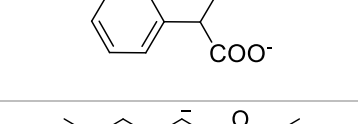
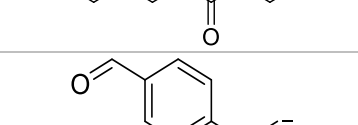
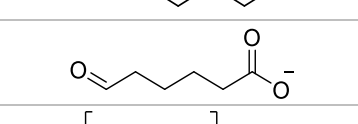
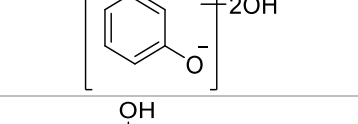
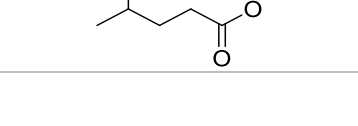
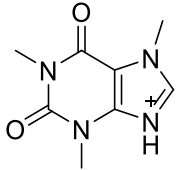
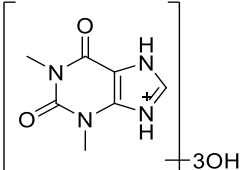
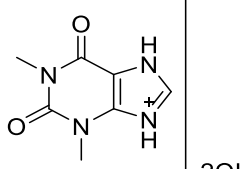
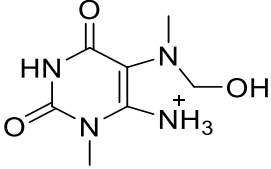
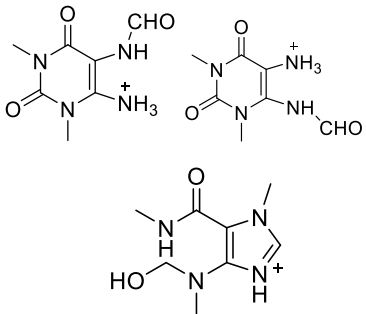
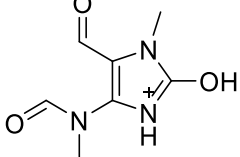
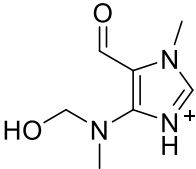
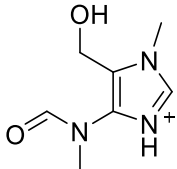
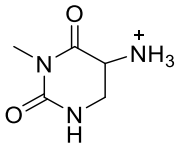
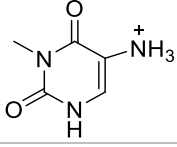
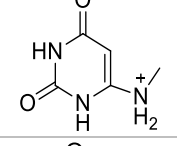
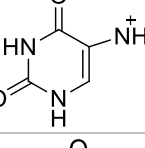
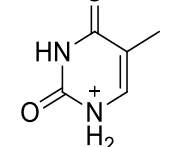
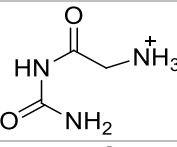
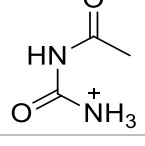
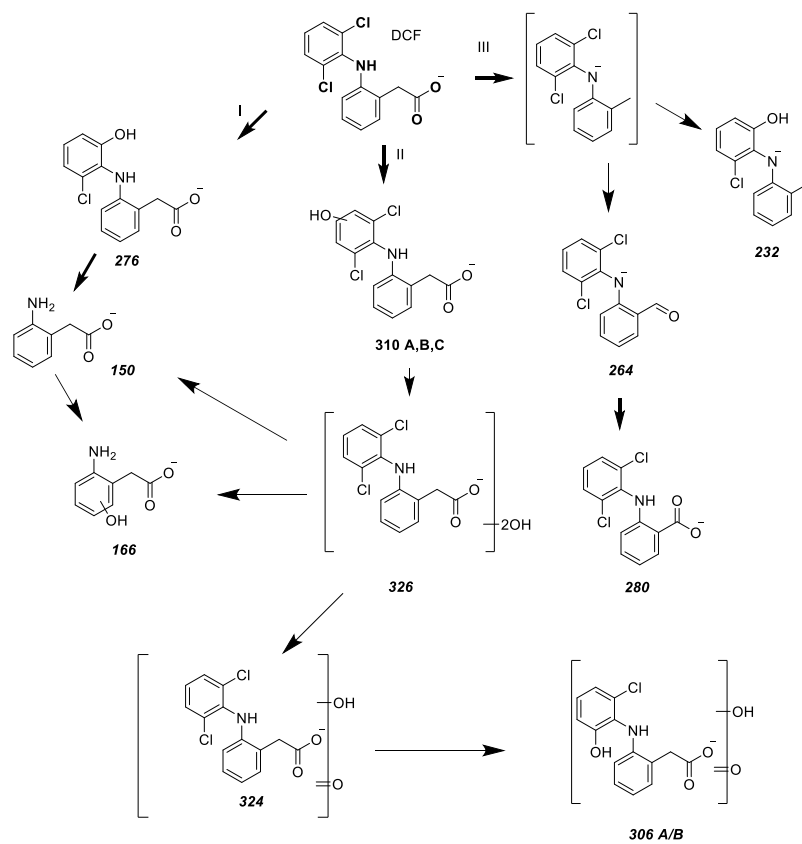
189.0907 C₁₂H₁₅O₂⁻	11.84	-		<i>This work</i>
181.0744 C₁₀H₁₃O₃⁻	1.93	-		<i>This work</i>
179.0743 C₁₀H₁₁O₃⁻	5.68	-		[13]
177.1274 C₁₂H₁₇O	A 8.53	163.1122 C ₁₁ H ₁₅ O ⁻ (- [*] CH ₃) [100]		[12]
	B 9.60	-		
165.0910 C₁₀H₁₃O₂⁻	16.66	150.0680 C ₉ H ₁₀ O ₂ ⁻ (- [*] CH ₃)		[14]
		93.0340 C ₆ H ₅ O ⁻ (-C ₄ H ₈ O)		
149.0631 C₉H₉O₂⁻	7.34	134.0365 C ₈ H ₆ O ₂ ⁻ (- [*] CH ₃)		[12]
		119.0487 C ₈ H ₇ O ⁻ (-CH ₂ O)		
143.1100 C₈H₁₅O₂⁻	13.26	-		<i>This work</i>
133.0681 C₉H₉O⁻	6.95	131.0489 C ₉ H ₇ O ⁻ (-H ₂)		[12, 13]
		105.0355 C ₈ H ₉ ⁻ (-CO)		
		103.0549 C ₈ H ₇ ⁻ (-H ₂ CO)		
129.0579 C₆H₉O₃⁻	5.89	-		[13]
125.0265 C₆H₅O₃⁻	2.79	-		<i>This work</i>
117.0546 C₅H₉O₃⁻	2.72	-		[13]

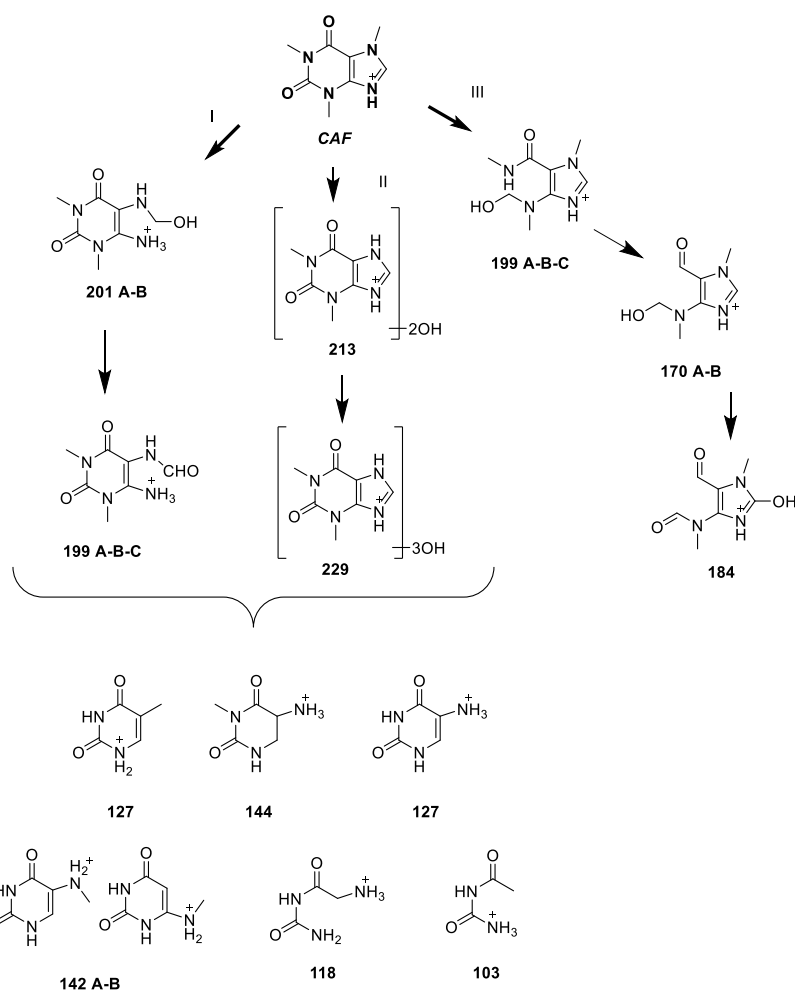
Table S15. Caffeine

Precursor ion [M+H] ⁺	t _R (min)	Product ions		Structure	Ref.
		MS ²	MS ³		
CAF 195.0876 C ₈ H ₁₁ N ₄ O ₂ ⁺	9.20	138.0660 (100) C ₆ H ₈ ON ₃ ⁺	110.0707 (100) C ₄ H ₈ N ₃ ⁺ (-CO)		[15]
			83.0597 (13) C ₄ H ₇ N ₂ (-C ₂ HON)		
			69.04414 (16) C ₃ H ₅ N ₂ (-C ₃ H ₃ ON)		
		181.0725 (0.11) C ₇ H ₉ N ₄ O ₂	-		
		110.0709 (1.33) C ₅ H ₈ N ₃	-		
		69.0442 (0.23) C ₃ H ₅ N ₂	-		
229.0934 C ₈ H ₁₃ N ₄ O ₄ ⁺	4.76	184.0666 C ₇ H ₁₀ N ₃ O ₃ ⁺ (-CH ₃ ON) [100]			This work
		211.0767 C ₈ H ₁₁ N ₄ O ₃ ⁺ (-H ₂ O) [5]			
213.0987 C ₈ H ₁₃ N ₄ O ₃ ⁺	4.25	186.0819 C ₇ H ₁₂ N ₃ O ₃ ⁺ (-CHN) [100]			This work
201.0985 C ₇ H ₁₃ N ₄ O ₃ ⁺	A 3.98	127.0463 C ₅ H ₇ N ₂ O ₂ ⁺ (-C ₂ H ₆ N ₂ O) [100]			This work
	B 5.78	170.0513 C ₆ H ₈ N ₃ O ₃ ⁺ (-CH ₅ N) [100]			
199.0824 C ₇ H ₁₁ N ₄ O ₃	A 2.90	-			[15]
	B 3.46	-			
	C 5.69	-			
184.0713 C ₇ H ₁₀ N ₃ O ₃ ⁺	5.27	156.0723 C ₆ H ₁₀ N ₃ O ₂ ⁺ (-CO) [100]			This work

170.0560 C₆H₈N₃O₃	A 5.50	153.0250 C ₆ H ₅ O ₃ N ₂ ⁺ (-NH ₃) [100]		<i>This work</i>
		96.0048 C ₄ H ₂ O ₂ N ⁺ (-C ₂ H ₆ N ₂ O) [18]		
	B 6.28	-		
144.0766 C₅H₁₀O₂N₃	3.68	127.0463 C ₅ H ₇ O ₂ N ₂ ⁺ (-NH ₃) [100]		[15]
		113.0093 C ₄ H ₅ N ₂ O ₂ ⁺ (-CH ₅ N) [32]		
142.0613 C₅H₈N₃O₂	A 4.54	57.0425 C ₂ H ₃ N ₂ ⁺ (-C ₃ H ₃ NO ₂) [100]		<i>This work</i>
	B 5.89	-		
128.0452 C₄H₆O₂N₃	3.68	-		<i>This work</i>
127.0499 C₅H₇N₂O₂	2.32	-		<i>This work</i>
118.0607 C₃H₈O₂N₃	3.65	-		<i>This work</i>
103.0497 C₃H₇O₂N₂	1.71	-		<i>This work</i>
				<i>This work</i>



Scheme 1S Transformation pathway of DCF in water.



Scheme 2S Main routes of CAF degradation in water.

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- [1] P. Calza, C. Medana, E. Padovano, V. Giancotti, C. Baiocchi, *Rapid Commun. Mass Spectrom.* 2012, **26**, 1687.
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