

Supplementary information

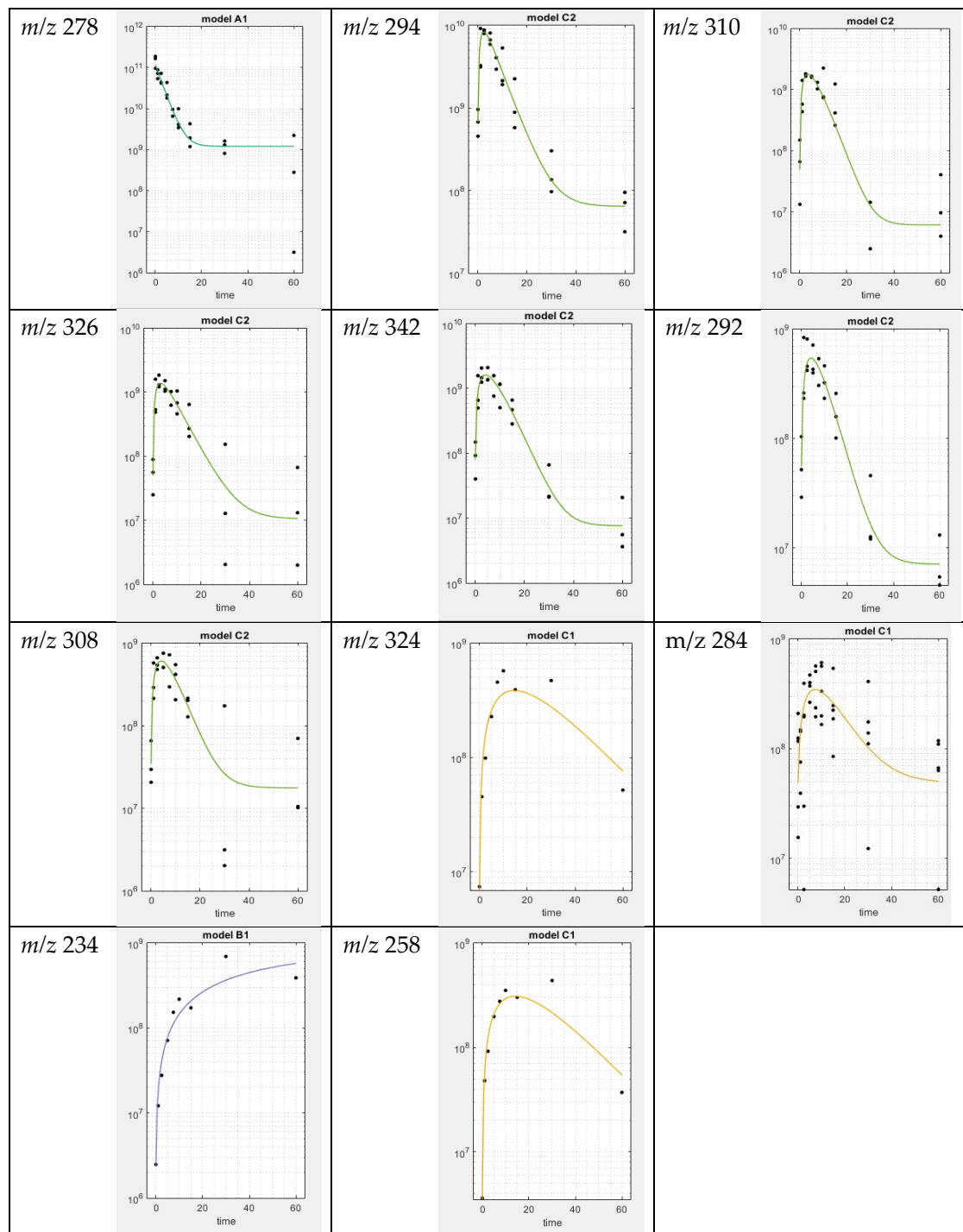
Comparison of advanced oxidation processes for the degradation of Maprotiline in water – kinetics, degradation products and potential ecotoxicity

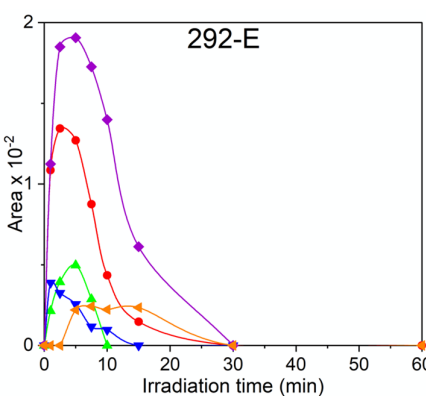
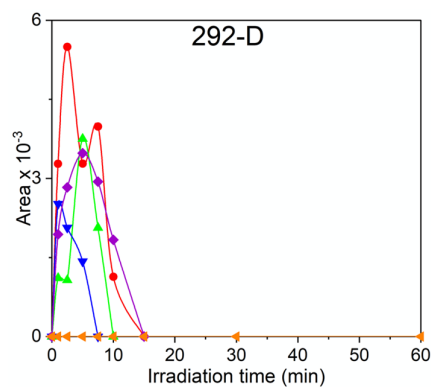
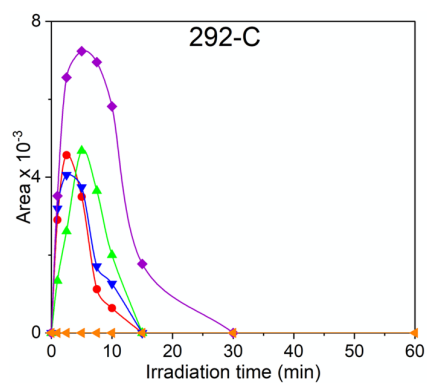
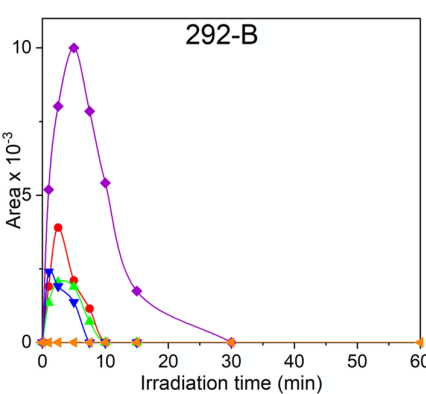
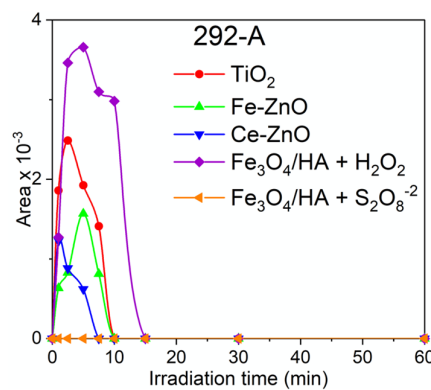
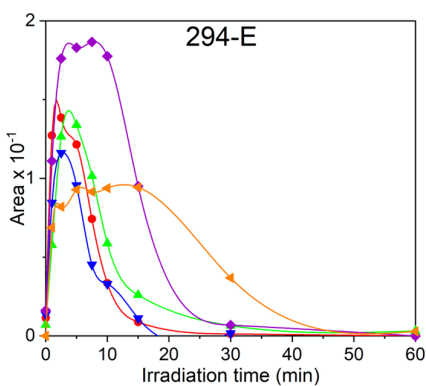
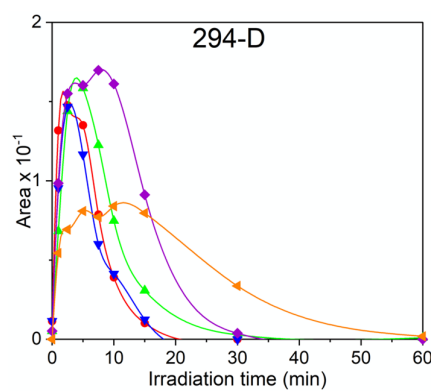
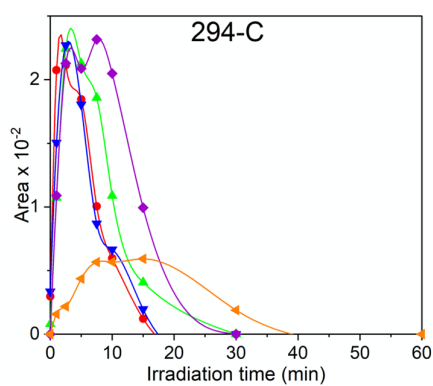
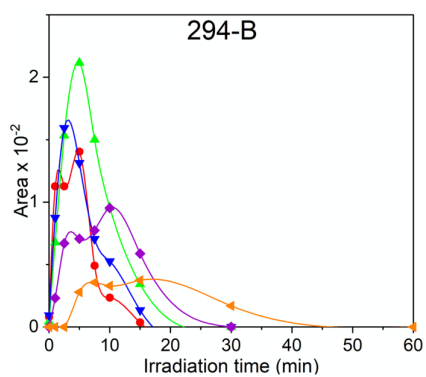
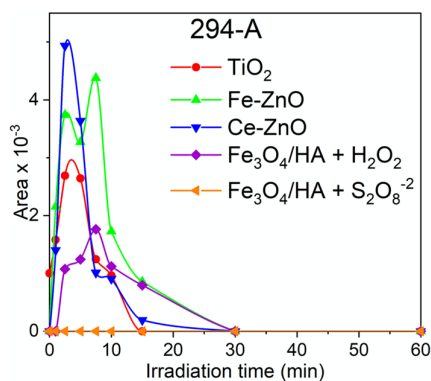
Nuno P.F Gonçalves^a, Zsuzsanna Varga^b, Edith Nicol^b, Paola Calza^a, Stéphane Bouchonnet^b

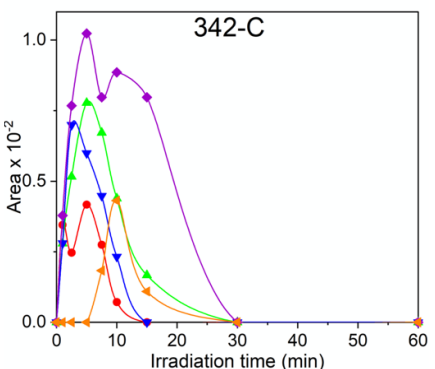
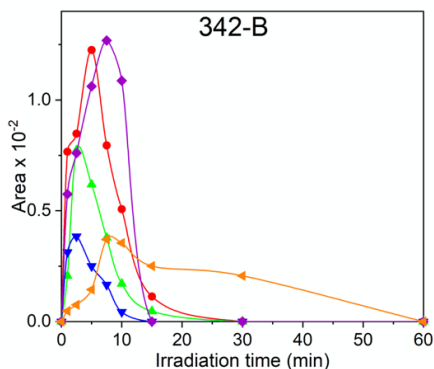
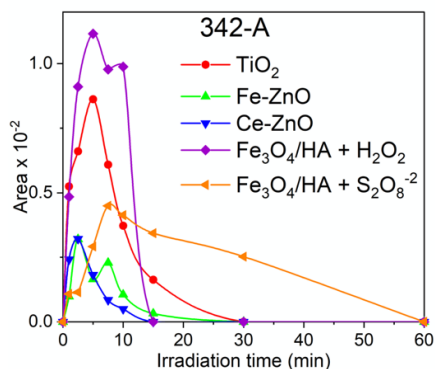
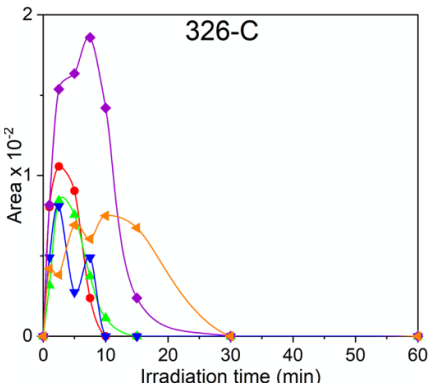
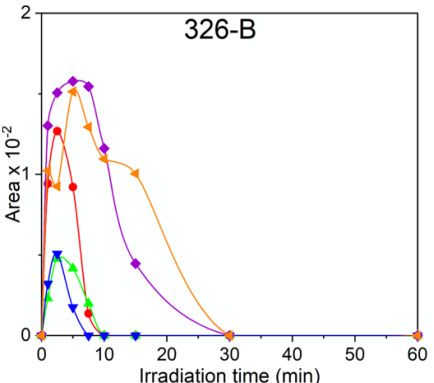
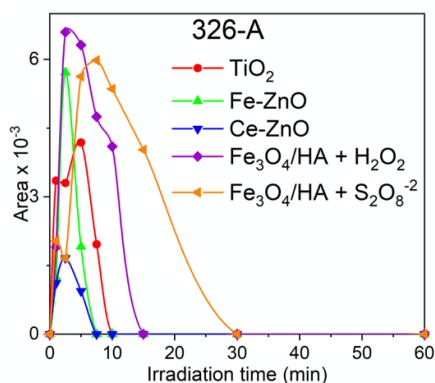
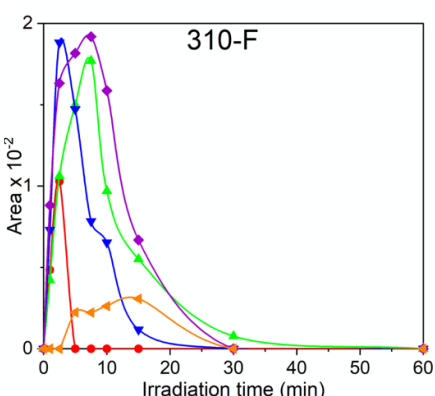
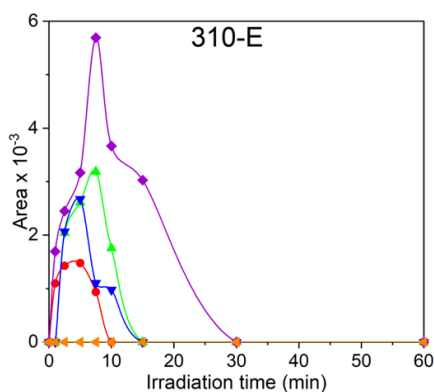
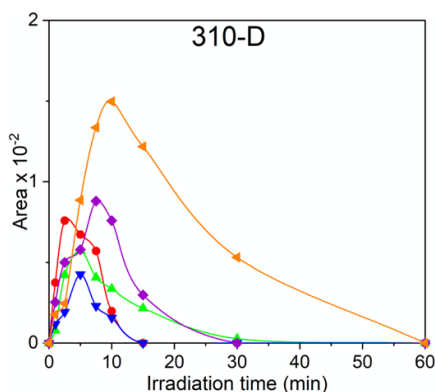
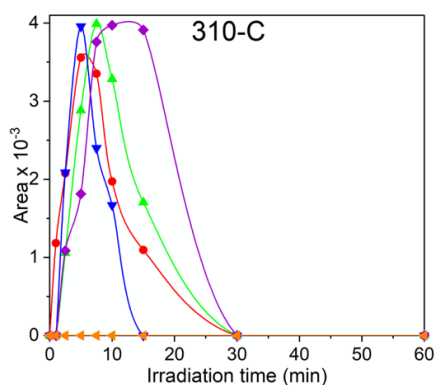
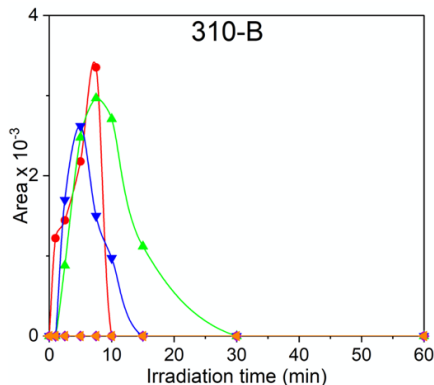
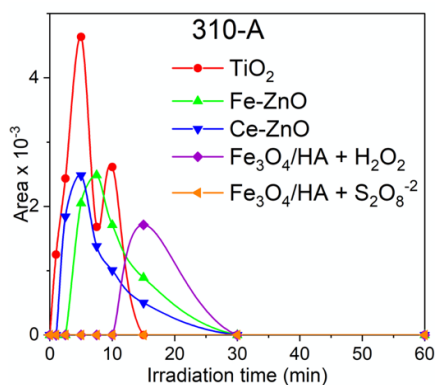
^aDepartment of Chemistry, University of Turin, Torino, Italy

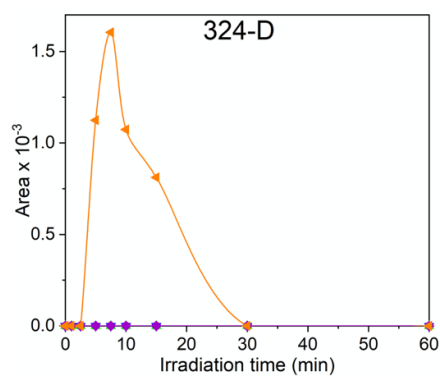
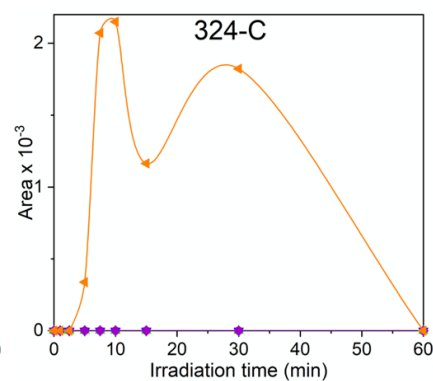
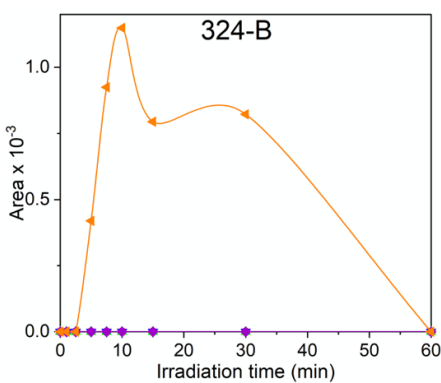
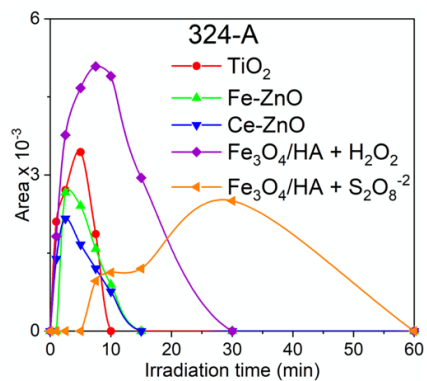
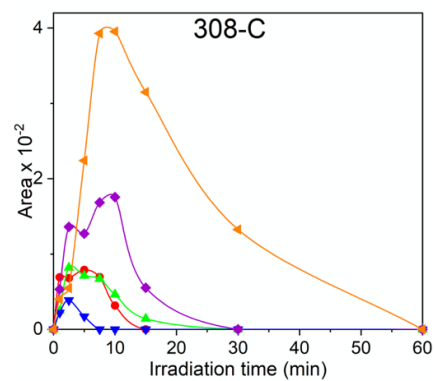
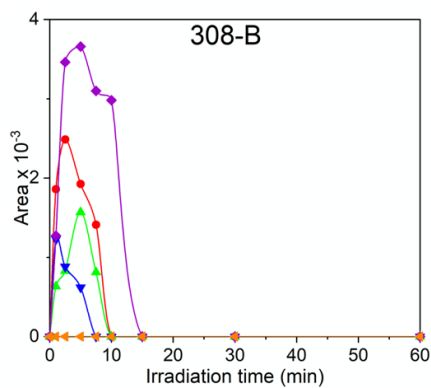
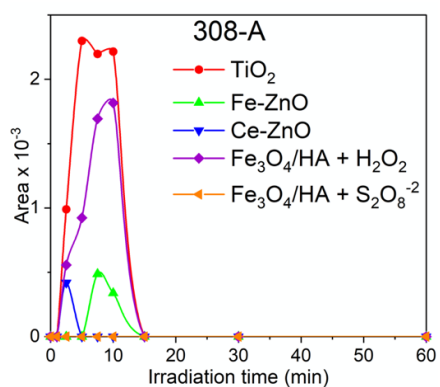
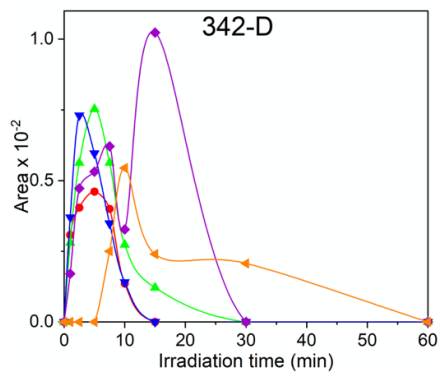
^bLaboratoire de Chimie Moléculaire - CNRS / Ecole Polytechnique, Institut Polytechnique de Paris, 91128, Palaiseau, France

Table S1. Summary of SPIX software output data from maprotiline and potential TP's









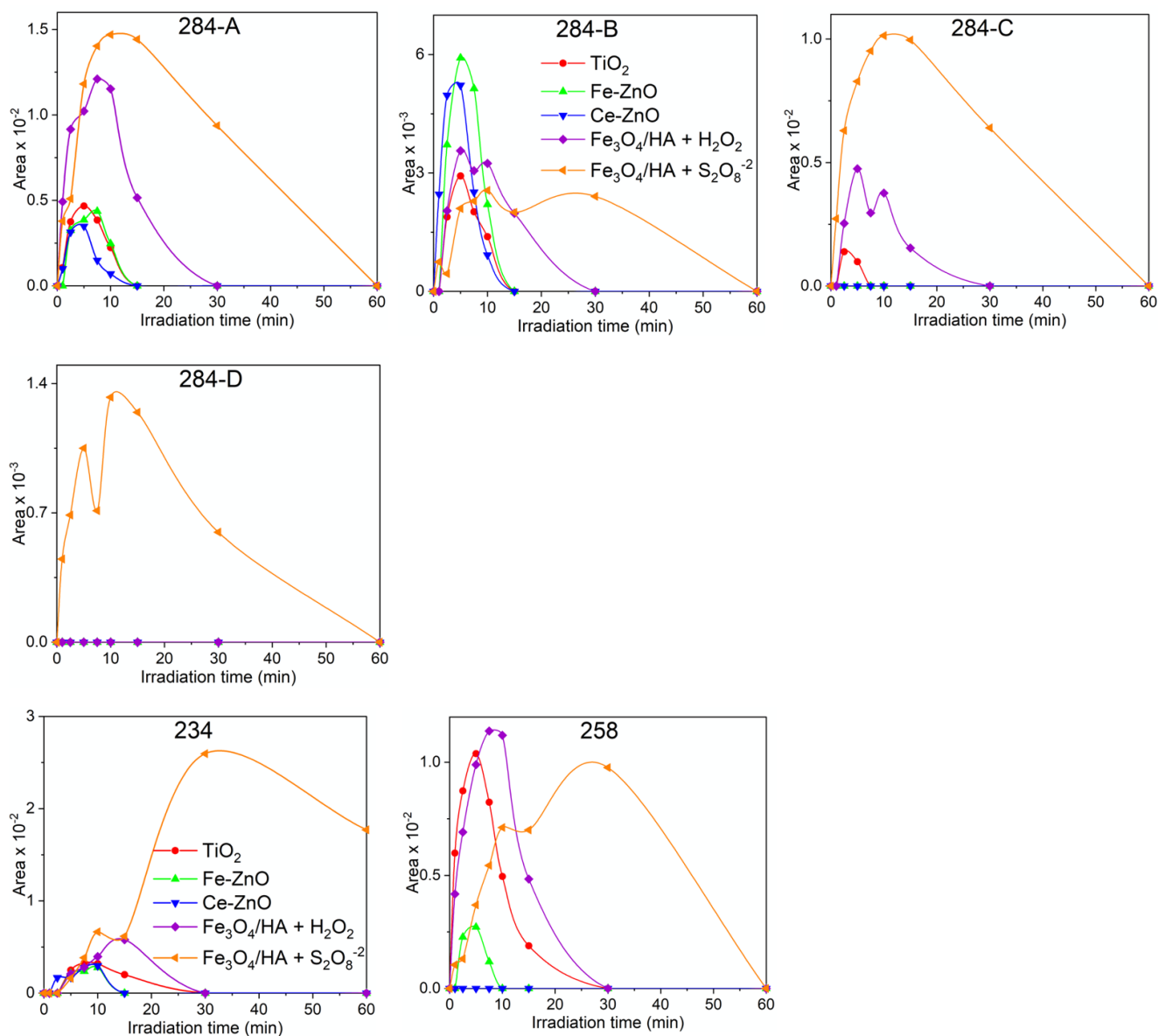


Figure S1. Evolution over time of maprotiline degradation products formed in the presence of different catalysts under UVA irradiation.

Table S2. Summary of $[M+H]^+$ and their main fragments from CDI experiments, together with the empirical formula.

Compound	$[M+H]^+$	Empirical Formula	Δ (ppm)	r.t. (min)	MS ²			Theoretical m/z
					m/z	Empirical formula	Δ (ppm)	
Maprotiline	278.1911	C ₂₀ H ₂₄ N	-2.81	9.7	278.19204	C ₂₀ H ₂₄ N	-6.2	278.19033
					250.16056	C ₁₈ H ₂₀ N	-6.2	250.15903
					219.11822	C ₁₇ H ₁₅	-6.4	219.11683
					169.10227	C ₁₃ H ₁₃	-6.5	169.10118
294-A	294.1858	C ₂₀ H ₂₄ NO	-1.98	7.3	294.18711	C ₂₀ H ₂₄ NO	-6.4	294.18524
					266.15559	C ₁₈ H ₂₀ NO	-6.2	266.15394
					235.11322	C ₁₇ H ₁₅ O	-6.3	235.11174
					217.10256	C ₁₇ H ₁₃	-6.4	217.10118
					207.08176	C ₁₅ H ₁₁ O	-6.4	207.08044
					191.08675	C ₁₅ H ₁₁	-6.4	191.08553
					157.06582	C ₁₁ H ₉ O	-6.5	157.06479
					117.07063	C ₉ H ₉	-6.4	117.06988

294-B					91.05479	C ₇ H ₇	-6.3	91.05423			
	7.8				276.17646	C ₂₀ H ₂₂ N	-6.5	276.17468			
					250.16060	C ₁₈ H ₂₀ N	-6.3	250.15903			
					245.13396	C ₁₉ H ₁₇	-6.0	245.13248			
					219.11823	C ₁₇ H ₁₅	-6.4	219.11683			
					217.10257	C ₁₇ H ₁₃	-6.4	217.10118			
					191.08675	C ₁₅ H ₁₁	-6.4	191.08553			
					141.07083	C ₁₁ H ₉	-6.8	141.06988			
					129.07073	C ₁₀ H ₉	-6.6	129.06988			
				91.05479	C ₇ H ₇	-6.3	91.05423				
294-C	8.0				294.18711	C ₂₀ H ₂₄ NO	-6.4	294.18524			
					266.15560	C ₁₈ H ₂₀ NO	-6.3	266.15394			
					235.11323	C ₁₇ H ₁₅ O	-6.3	235.11174			
					209.09744	C ₁₅ H ₁₃ O	-6.4	209.09609			
					207.08176	C ₁₅ H ₁₁ O	-6.4	207.08044			
					185.09729	C ₁₃ H ₁₃ O	-6.5	185.09609			
					169.10226	C ₁₃ H ₁₃	-6.4	169.10118			
					147.08137	C ₁₀ H ₁₁ O	-6.3	147.08044			
					143.08648	C ₁₁ H ₁₁	-6.7	143.08553			
					133.06565	C ₉ H ₉ O	-6.5	133.06479			
					117.07063	C ₉ H ₉	-6.4	117.06988			
					107.04981	C ₇ H ₇ O	-6.2	107.04914			
				91.05480	C ₇ H ₇	-6.3	91.05423				
294-D	8.3				294.18705	C ₂₀ H ₂₄ NO	-6.2	294.18524			
					266.15560	C ₁₈ H ₂₀ NO	-6.2	266.15394			
					263.14469	C ₁₉ H ₁₉ O	-6.3	263.14304			
					245.13404	C ₁₉ H ₁₇	-6.4	245.13248			
					235.11322	C ₁₇ H ₁₅ O	-6.3	235.11174			
					221.09751	C ₁₆ H ₁₃ O	-6.4	221.09609			
					217.10256	C ₁₇ H ₁₃	-6.4	217.10118			
					209.09743	C ₁₅ H ₁₃ O	-6.4	209.09609			
					207.08177	C ₁₅ H ₁₁ O	-6.5	207.08044			
					185.09730	C ₁₃ H ₁₃ O	-6.5	185.09609			
					169.10228	C ₁₃ H ₁₃	-6.5	169.10118			
					143.08646	C ₁₁ H ₁₁	-6.5	143.08553			
					141.07079	C ₁₁ H ₉	-6.5	141.06988			
					133.06565	C ₉ H ₉ O	-6.5	133.06479			
					129.07071	C ₁₀ H ₉	-6.5	129.06988			
					117.07063	C ₉ H ₉	-6.5	117.06988			
					107.04982	C ₇ H ₇ O	-6.4	107.04914			
				91.05479	C ₇ H ₇	-6.3	91.05423				
294-E	8.9				294.18705	C ₂₀ H ₂₄ NO	-6.2	294.18524			
					276.17642	C ₂₀ H ₂₂ N	-6.3	276.17468			
					266.15560	C ₁₈ H ₂₀ NO	-6.2	266.15394			
					235.11323	C ₁₇ H ₁₅ O	-6.3	235.11174			
					217.10257	C ₁₇ H ₁₃	-6.4	217.10118			
					207.08177	C ₁₅ H ₁₁ O	-6.4	207.08044			
					185.09729	C ₁₃ H ₁₃ O	-6.5	185.09609			
					169.10228	C ₁₃ H ₁₃	-6.5	169.10118			
					157.06581	C ₁₁ H ₉ O	-6.5	157.06479			
					141.07079	C ₁₁ H ₉	-6.5	141.06988			
					133.06565	C ₉ H ₉ O	-6.5	133.06479			
					117.07063	C ₉ H ₉	-6.5	117.06988			
					107.04982	C ₇ H ₇ O	-6.4	107.04914			
					91.05479	C ₇ H ₇	-6.3	91.05423			
	310-A	310.1807	C ₂₀ H ₂₄ NO ₂	-2.00	6.9				310.18204	C ₂₀ H ₂₄ NO ₂	-6.1
								292.17139	C ₂₀ H ₂₂ NO	-6.2	292.16959
								279.13967	C ₁₉ H ₁₉ O ₂	-6.2	279.13796
								261.12902	C ₁₉ H ₁₇ O	-6.3	261.12739
								217.10256	C ₁₇ H ₁₃	-6.4	217.10118
								191.08676	C ₁₅ H ₁₁	-6.5	191.08553
								185.09729	C ₁₃ H ₁₃ O	-6.5	185.09609
								159.08147	C ₁₁ H ₁₁ O	-6.5	159.08044

310-B	7.2	133.06565	C ₉ H ₉ O	-6.5	133.06479				
		310.18203	C ₂₀ H ₂₄ NO ₂	-6.1	310.18016				
		292.17138	C ₂₀ H ₂₂ NO	-6.1	292.16959				
		266.15562	C ₁₈ H ₂₀ NO	-6.3	266.15394				
		261.12903	C ₁₉ H ₁₇ O	-6.3	261.12739				
		233.09758	C ₁₇ H ₁₃ O	-6.4	233.09609				
		207.08177	C ₁₅ H ₁₁ O	-6.5	207.08044				
		169.10228	C ₁₃ H ₁₃	-6.5	169.10118				
		141.07079	C ₁₁ H ₉	-6.5	141.06988				
		123.04485	C ₇ H ₇ O ₂	-6.5	123.04406				
310-C	7.4	89.06026	C ₄ H ₉ O ₂	-6.2	89.05971				
		310.18204	C ₂₀ H ₂₄ NO ₂	-6.1	310.18016				
		282.15060	C ₁₈ H ₂₀ NO ₂	-6.2	282.14886				
		279.13967	C ₁₉ H ₁₉ O ₂	-6.2	279.13796				
		251.10824	C ₁₇ H ₁₅ O ₂	-6.3	251.10666				
		185.09729	C ₁₃ H ₁₃ O	-6.5	185.09609				
		159.08147	C ₁₁ H ₁₁ O	-6.5	159.08044				
		145.06574	C ₁₀ H ₉ O	-6.6	145.06479				
		133.06565	C ₉ H ₉ O	-6.5	133.06479				
		107.04983	C ₇ H ₇ O	-6.4	107.04914				
310-D	8.0	310.18204	C ₂₀ H ₂₄ NO ₂	-6.1	310.18016				
		282.15060	C ₁₈ H ₂₀ NO ₂	-6.2	282.14886				
		251.10824	C ₁₇ H ₁₅ O ₂	-6.3	251.10666				
		233.09756	C ₁₇ H ₁₃ O	-6.3	233.09609				
		201.09230	C ₁₃ H ₁₃ O ₂	-6.4	201.09101				
		169.10227	C ₁₃ H ₁₃	-6.5	169.10118				
		143.08646	C ₁₁ H ₁₁	-6.5	143.08553				
		141.07079	C ₁₁ H ₉	-6.5	141.06988				
310-E	8.2	310.18206	C ₂₀ H ₂₄ NO ₂	-6.1	310.18016				
		292.17138	C ₂₀ H ₂₂ NO	-6.1	292.16959				
		280.13493	C ₁₈ H ₁₈ NO ₂	-6.2	280.13321				
		233.09760	C ₁₇ H ₁₃ O	-6.5	233.09609				
		101.06036	C ₅ H ₉ O ₂	-6.5	101.05971				
310-F	8.4	310.18204	C ₂₀ H ₂₄ NO ₂	-6.1	310.18016				
		250.16058	C ₁₈ H ₂₀ N	-6.2	250.15903				
		217.10256	C ₁₇ H ₁₃	-6.4	217.10118				
		191.08676	C ₁₅ H ₁₁	-6.5	191.08553				
326-A	326.1757	C ₂₀ H ₂₄ NO ₃	-2.13	6.1	326.17702	C ₂₀ H ₂₄ NO ₃	-6.0	326.17507	
					308.16641	C ₂₀ H ₂₂ NO ₂	-6.2	308.16451	
					298.14555	C ₁₈ H ₂₀ NO ₃	-6.0	298.14377	
					185.09729	C ₁₃ H ₁₃ O	-6.5	185.09609	
					89.06025	C ₄ H ₉ O ₂	-6.2	89.059706	
326-B					6.9	326.17702	C ₂₀ H ₂₄ NO ₃	-6.0	326.17507
					308.16635	C ₂₀ H ₂₂ NO ₂	-6.0	308.16451	
					298.14556	C ₁₈ H ₂₀ NO ₃	-6.0	298.14377	
					267.10324	C ₂₀ H ₁₃ N	3.8	267.10425	
					191.08674	C ₁₅ H ₁₁	-6.4	191.08553	
					185.09728	C ₁₃ H ₁₃ O	-6.4	185.09609	
326-C	7.6	326.17698	C ₂₀ H ₂₄ NO ₃	-5.9	326.17507				
		308.16636	C ₂₀ H ₂₂ NO ₂	-6.0	308.16451				
		298.14556	C ₁₈ H ₂₀ NO ₃	-6.0	298.14377				
		298.14556	C ₁₈ H ₂₀ NO ₃	-6.0	298.14377				
		280.13492	C ₁₈ H ₁₈ NO ₂	-6.1	280.13321				
		267.10320	C ₂₀ H ₁₃ N	3.9	267.10425				
		249.09256	C ₁₇ H ₁₃ O ₂	-6.2	249.09101				
342-A	342.1707	C ₂₀ H ₂₄ NO ₄	-2.09	6.0	342.17199	C ₂₀ H ₂₄ NO ₄	-5.9	342.16999	
					324.16134	C ₂₀ H ₂₂ NO ₃	-5.9	324.15942	
					275.10835	C ₁₉ H ₁₅ O ₂	-6.2	275.10666	
					247.07691	C ₁₇ H ₁₁ O ₂	-6.3	247.07536	
					183.08162	C ₁₃ H ₁₁ O	-6.4	183.08044	
342-B					6.4	342.17199	C ₂₀ H ₂₄ NO ₄	-5.9	342.16999
					324.16134	C ₂₀ H ₂₂ NO ₃	-5.9	324.15942	

342-C					306.15070	C ₂₀ H ₂₀ NO ₂	-6.0	306.14886	
					216.13965	C ₁₄ H ₁₈ NO	-6.3	216.13829	
					185.09729	C ₁₃ H ₁₃ O	-6.4	185.09609	
					167.08662	C ₁₃ H ₁₁	-6.5	167.08553	
					157.06581	C ₁₁ H ₉ O	-6.5	157.06479	
					7.1	342.17199	C ₂₀ H ₂₄ NO ₄	-5.8	342.16999
					324.16136	C ₂₀ H ₂₂ NO ₃	-6.0	324.15942	
					296.16630	C ₁₉ H ₂₂ NO ₂	-6.1	296.16451	
					240.13980	C ₁₆ H ₁₈ NO	-6.3	240.13829	
					133.08678	C ₆ H ₁₃ O ₃	-6.4	133.08592	
342-D					89.06025	C ₄ H ₉ O ₂	-6.1	89.05971	
					7.6	342.17198	C ₂₀ H ₂₄ NO ₄	-5.8	342.16999
					324.16135	C ₂₀ H ₂₂ NO ₃	-6.0	324.15942	
					296.16632	C ₁₉ H ₂₂ NO ₂	-6.1	296.16451	
					240.13981	C ₁₆ H ₁₈ NO	-6.3	240.13829	
					212.14474	C ₁₅ H ₁₈ N	-6.4	212.14338	
292-A	292.1701	C ₂₀ H ₂₂ NO	-2.06	6.9	292.17143	C ₂₀ H ₂₂ NO	-6.3	292.16959	
					250.16059	C ₁₈ H ₂₀ N	-6.3	250.15903	
					217.10255	C ₁₇ H ₁₃	-6.3	217.10118	
					191.08676	C ₁₅ H ₁₁	-6.5	191.08553	
292-B				7.9	292.17137	C ₂₀ H ₂₂ NO	-6.1	292.16959	
					250.16059	C ₁₈ H ₂₀ N	-6.3	250.15903	
					219.11816	C ₁₇ H ₁₅	-6.1	219.11683	
					191.08674	C ₁₅ H ₁₁	-6.3	191.08553	
292-C				8.5	292.17137	C ₂₀ H ₂₂ NO	-6.1	292.16959	
					250.16058	C ₁₈ H ₂₀ N	-6.2	250.15903	
					243.11832	C ₁₉ H ₁₅	-6.2	243.11683	
					219.11822	C ₁₇ H ₁₅	-6.3	219.11683	
292-D				8.8	191.08674	C ₁₅ H ₁₁	-6.4	191.08553	
					292.17134	C ₂₀ H ₂₂ NO	-6.0	292.16959	
					243.11833	C ₁₉ H ₁₅	-6.2	243.11683	
					217.10255	C ₁₇ H ₁₃	-6.3	217.10118	
292-E				9.1	191.08676	C ₁₅ H ₁₁	-6.4	191.08553	
					292.17143	C ₂₀ H ₂₂ NO	-6.3	292.16959	
					246.12921	C ₁₈ H ₁₆ N	-6.0	246.12773	
308-A	308.1651	C ₂₀ H ₂₂ NO ₂	-1.96	6.4	183.08162	C ₁₃ H ₁₁ O	-6.4	183.08044	
					308.1664	C ₂₀ H ₂₂ NO ₂	-6.2	308.16451	
					233.09756	C ₁₇ H ₁₃ O	-6.3	233.09609	
					215.08689	C ₁₇ H ₁₁	-6.4	215.08553	
					207.08176	C ₁₅ H ₁₁ O	-6.4	207.08044	
308-B				7.3	203.08682	C ₁₆ H ₁₁	-6.4	203.08553	
					308.16636	C ₂₀ H ₂₂ NO ₂	-6.0	308.16451	
					265.14775	C ₁₈ H ₁₉ NO	-6.2	265.14612	
					233.09756	C ₁₇ H ₁₃ O	-6.3	233.09609	
					215.08688	C ₁₇ H ₁₁	-6.3	215.08553	
					207.08176	C ₁₅ H ₁₁ O	-6.4	207.08044	
308-C				7.7	178.07885	C ₁₄ H ₁₀	-6.4	178.07770	
					308.16633	C ₂₀ H ₂₂ NO ₂	-5.9	308.16451	
324-A	324.1599	C ₂₀ H ₂₂ NO ₃	-1.70	5.8	280.13492	C ₁₈ H ₁₈ NO ₂	-6.1	280.13321	
					324.16135	C ₂₀ H ₂₂ NO ₃	-6.0	324.15942	
					306.15069	C ₂₀ H ₂₀ NO ₂	-6.0	306.14886	
					247.13711	C ₁₈ H ₁₇ N	-6.3	247.13555	
					233.09758	C ₁₇ H ₁₃ O	-6.4	233.09609	
					207.08177	C ₁₅ H ₁₁ O	-6.4	207.08044	
324-B				6.4	191.08674	C ₁₅ H ₁₁	-6.3	191.08553	
					324.16131	C ₂₀ H ₂₂ NO ₃	-5.8	324.15942	
					296.12993	C ₁₈ H ₁₈ NO ₃	-6.1	296.12812	
					249.09256	C ₁₇ H ₁₃ O ₂	-6.2	249.09101	
324-C				7.0	110.09711	C ₇ H ₁₂ N	-6.2	110.09643	
					324.16131	C ₂₀ H ₂₂ NO ₃	-5.8	324.15942	
					296.12992	C ₁₈ H ₁₈ NO ₃	-6.1	296.12812	
					265.08750	C ₂₀ H ₁₁ N	4.2	265.08860	

324-D					7.9	324.16134	C ₂₀ H ₂₂ NO ₃	-5.9	324.15942
						293.11810	C ₁₉ H ₁₇ O ₃	-6.1	293.11722
						265.08756	C ₂₀ H ₁₁ N	3.9	265.08860
284-A	284.1650	C ₁₈ H ₂₂ NO ₅	-1.75	6.7	284.16624	C ₁₈ H ₂₂ NO ₂	-6.1	284.16451	
					253.12389	C ₁₇ H ₁₇ O ₂	-6.3	253.12231	
					225.12883	C ₁₆ H ₁₇ O	-6.4	225.12739	
284-B				7.3	284.16635	C ₁₈ H ₂₂ NO ₂	-6.5	284.16451	
					89.06026	C ₄ H ₉ O ₂	-6.2	89.05971	
284-C				7.7	284.16624	C ₁₈ H ₂₂ NO ₂	-6.1	284.16451	
					256.13479	C ₁₆ H ₁₈ NO ₂	-6.2	256.13321	
					225.09242	C ₁₅ H ₁₃ O ₂	-6.3	225.09101	
284-D				8.4	284.16618	C ₁₈ H ₂₂ NO ₂	-5.9	284.16451	
					256.13481	C ₁₆ H ₁₈ NO ₂	-6.3	256.13321	
					238.12416	C ₁₆ H ₁₆ NO	-6.4	238.12264	
					89.06026	C ₄ H ₉ O ₂	-6.2	89.05971	
234	234.1492	C ₁₄ H ₂₀ NO ₂	-1.70	4.4					
258	258.1493	C ₁₆ H ₂₀ NO ₂	-1.77	6.3	258.15046	C ₁₆ H ₂₀ NO ₂	-6.2	258.14886	
					240.13980	C ₁₆ H ₁₈ NO	-6.3	240.13829	
					212.14473	C ₁₅ H ₁₈ N	-6.4	212.14338	