SUPPLEMENTARY INFORMATION

Influence of electron acceptors on the kinetics of metoprolol photocatalytic degradation in TiO_2 suspension. A combined experimental and theoretical study

S. J. Armaković,[a] S. Armaković,[b] N. L. Finčur,[a] F. Šibul,[a] D. Vione,[c] J. P. Šetrajčić[b] and B. F. Abramović[a,*]

[a] Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, Trg D. Obradovića 3, 21000 Novi Sad, Serbia
[b] Department of Physics, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 4, 21000 Novi Sad, Serbia
[c] Dipartimento di Chimica, Università di Torino, Via Pietro Giuria 5, 10125 Torino, Italy

*Corresponding Author
E-mail: biljana.abramovic@dh.uns.ac.rs

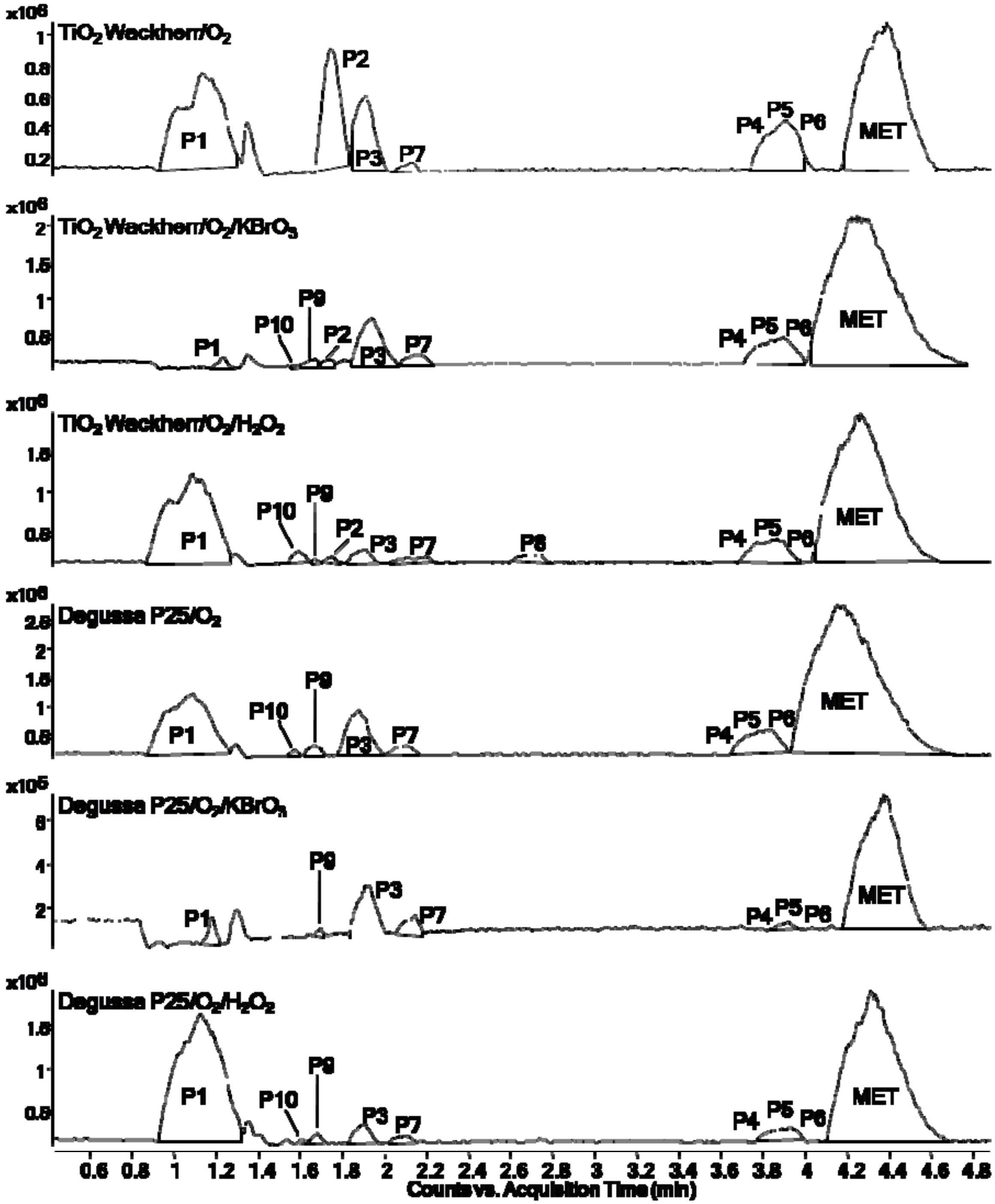

Fig. S1. Base peak chromatograms of metoprolol (MET) in presence of TiO_2 Wackherr or Degussa P25, with different electron acceptors, in positive mode.

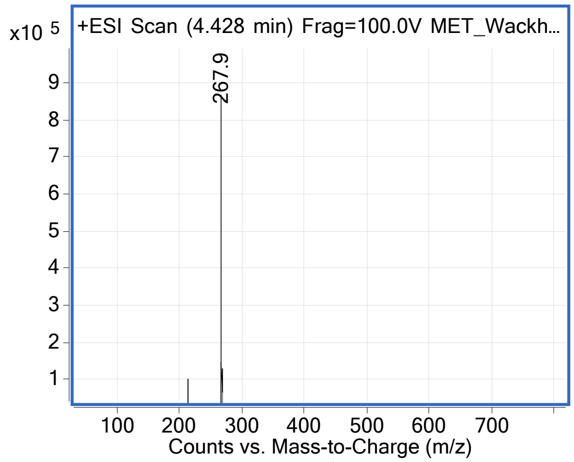

Fig. S2. Positive mode MS^1 spectra of MET.

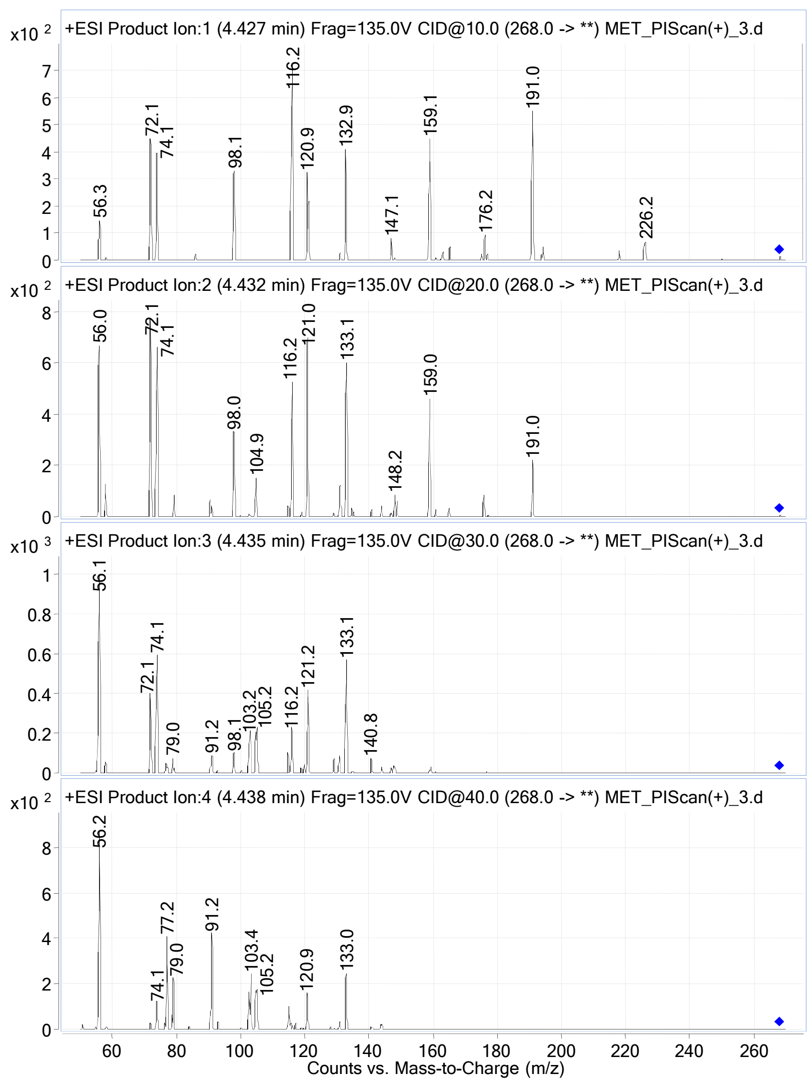

Fig. S3. Positive mode MS^2 spectra of MET.

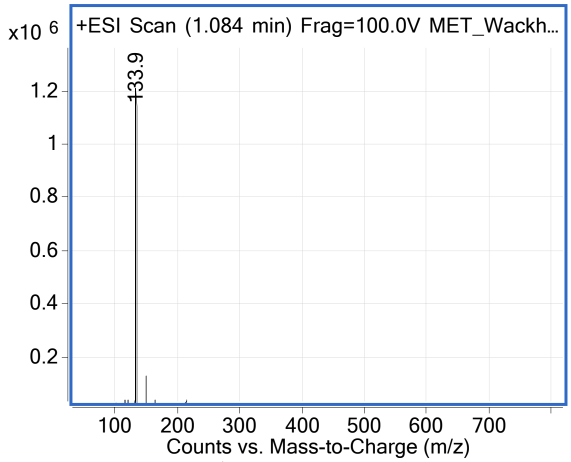

Fig. S4. Positive mode MS^1 spectra of degradation product P1.

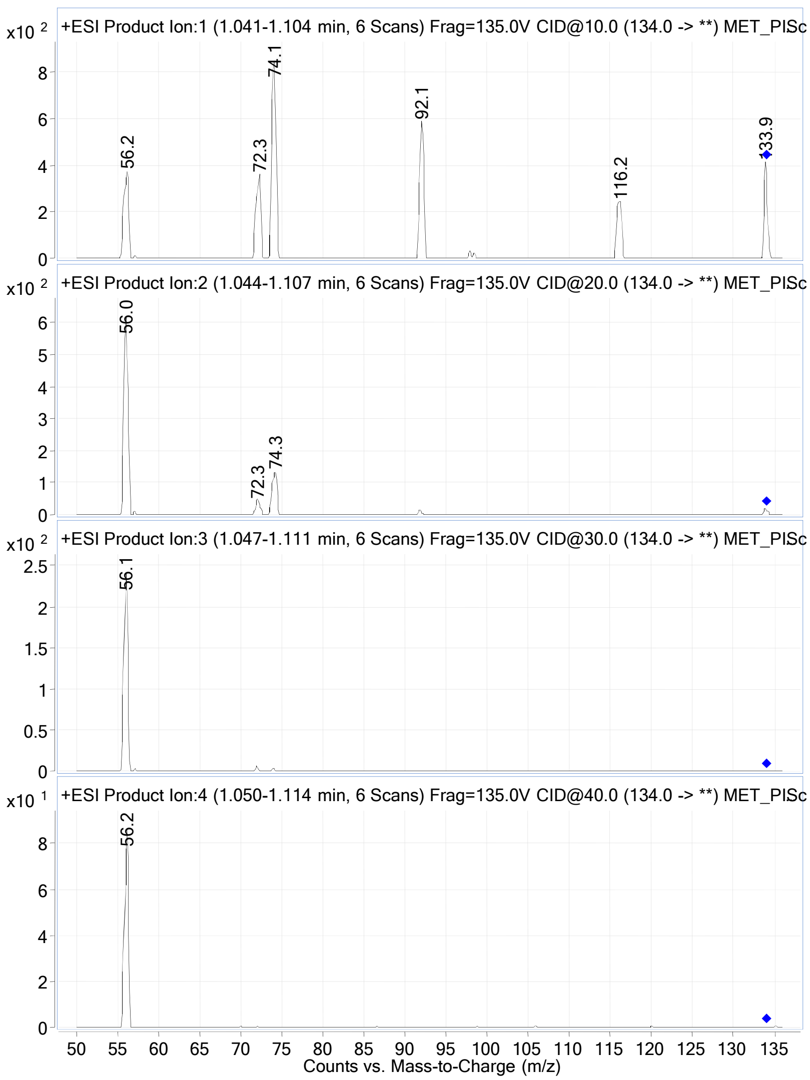

Fig. S5. Positive mode MS^2 spectra of degradation product P1.

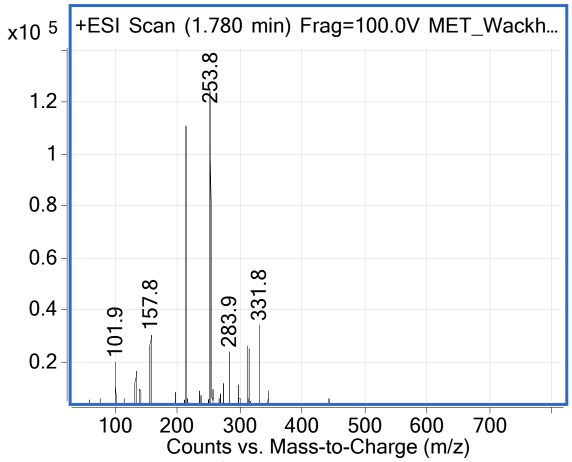

Fig. S6. Positive mode MS^1 spectra of degradation product P2.

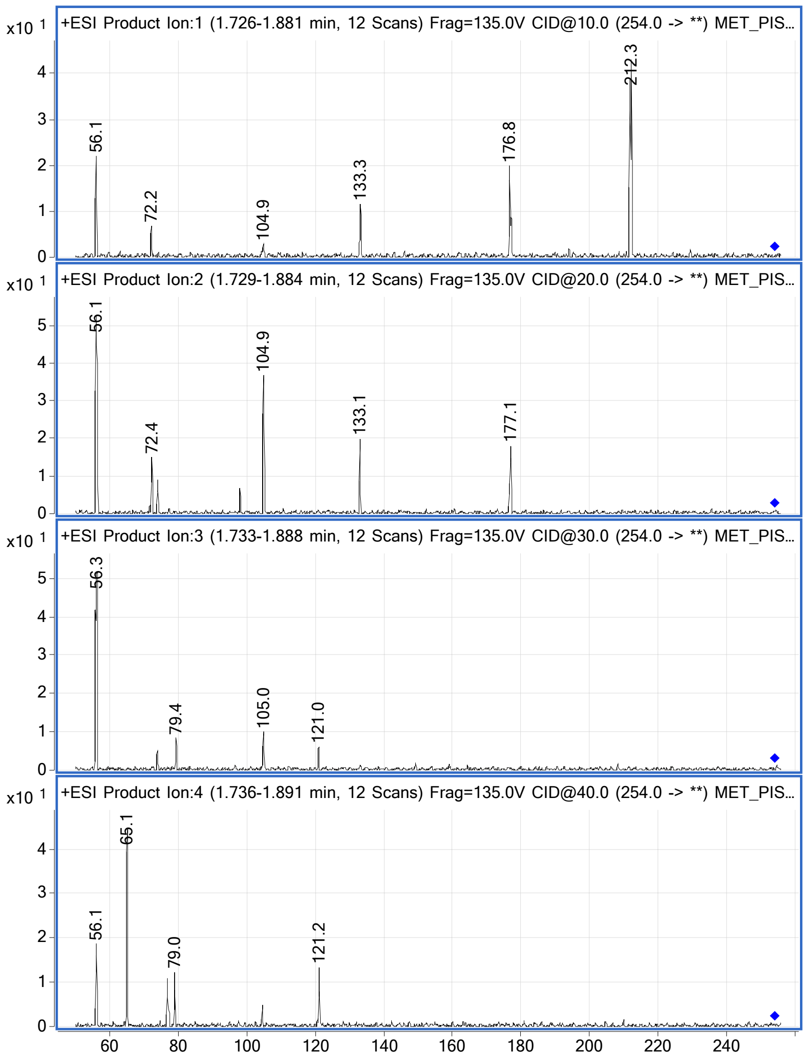

Fig. S7. Positive mode MS^2 spectra of degradation product P2.

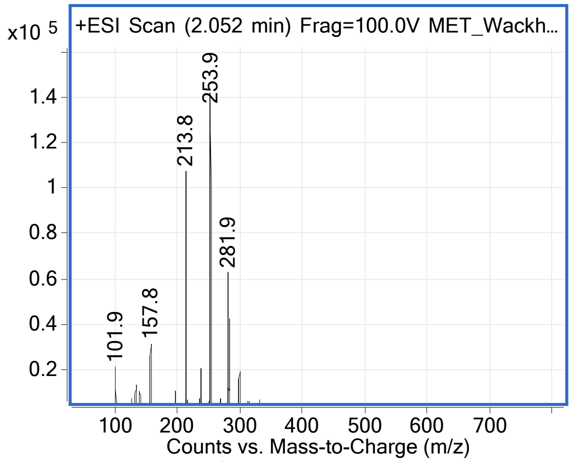

Fig. S8. Positive mode MS^1 spectra of degradation product P3.

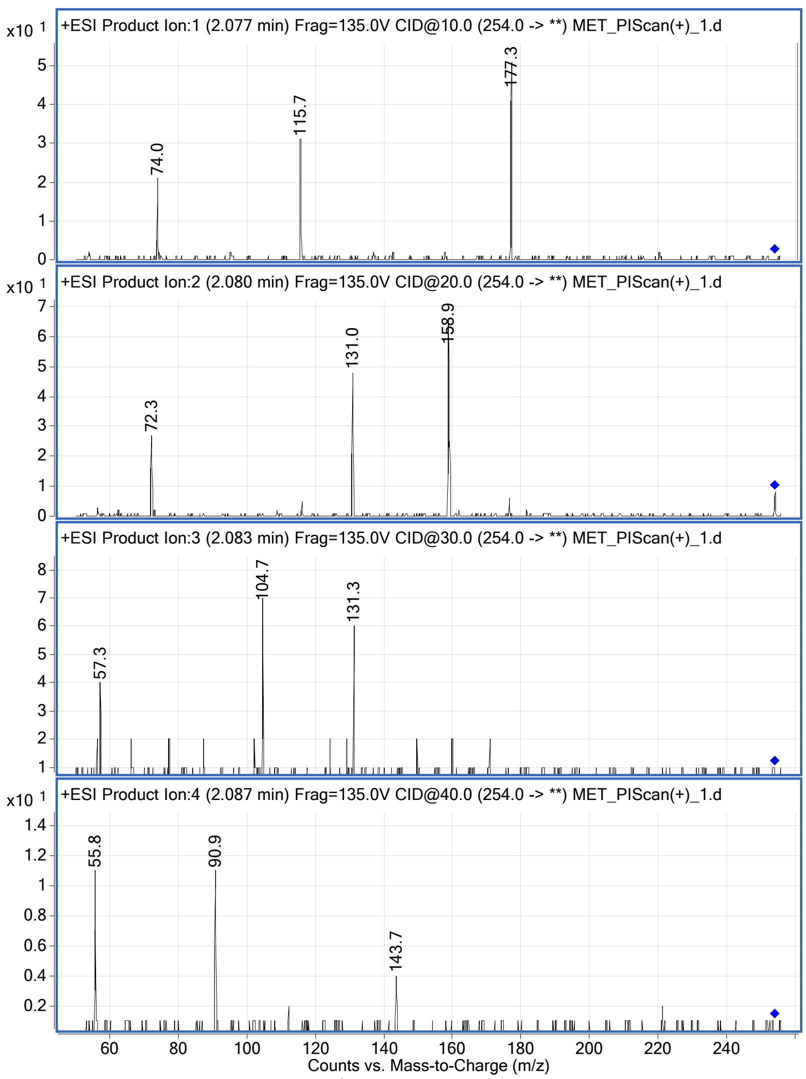

Fig. S9. Positive mode MS^2 spectra of degradation product P3.

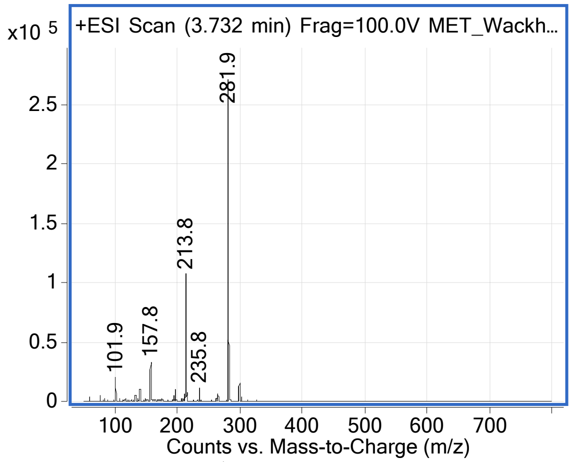

Fig. S10. Positive mode MS[1] spectra of degradation product P4a.

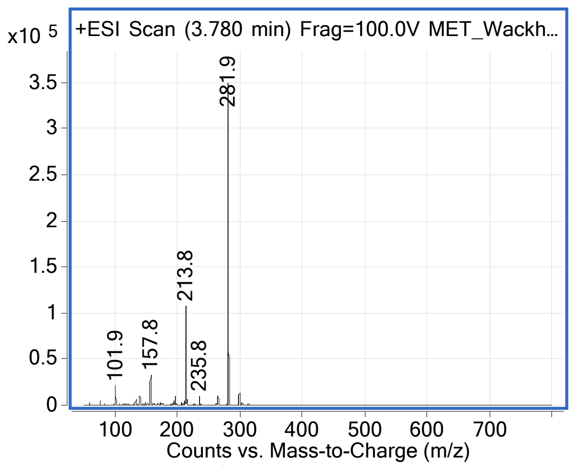

Fig. S11. Positive mode MS[1] spectra of degradation product P4b.

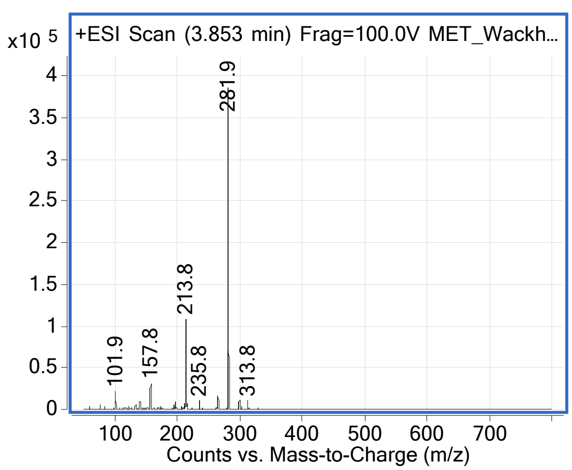

Fig. S12. Positive mode MS[1] spectra of degradation product P5.

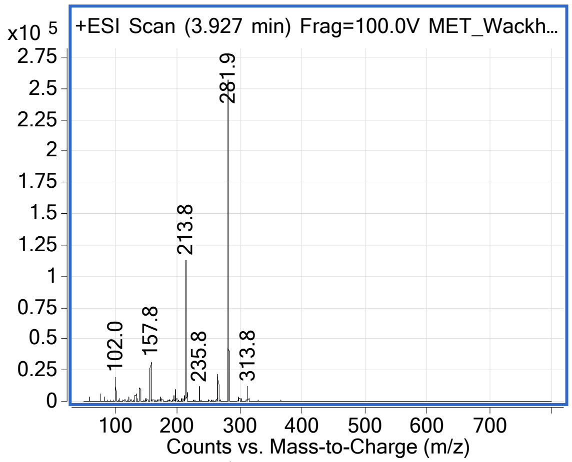

Fig. S13. Positive mode MS[1] spectra of degradation product P6.

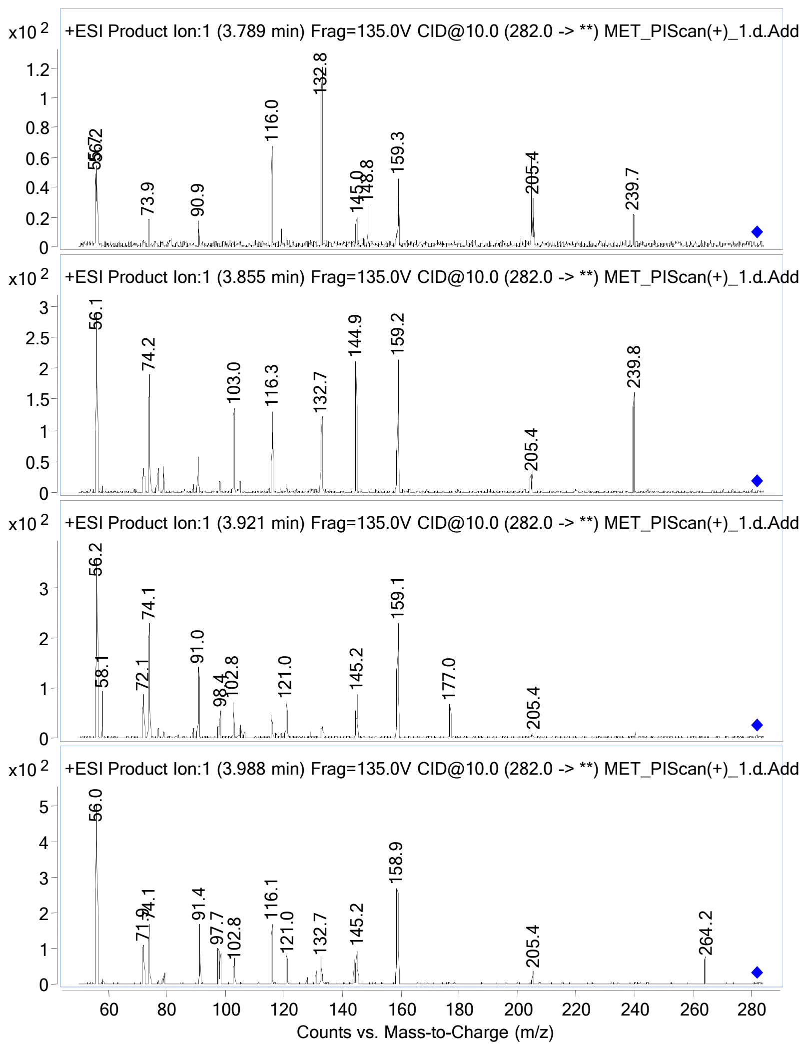

Fig. S14. Positive mode composite MS[2] spectra of degradation products P4a, P4b, P5 and P6, respectively.

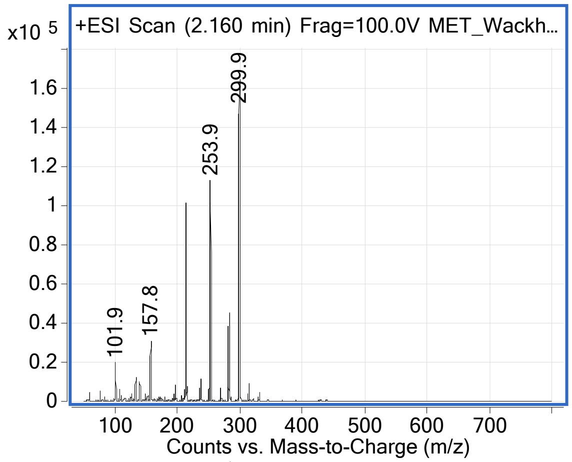

Fig. S15. Positive mode MS^1 spectra of degradation product P7.

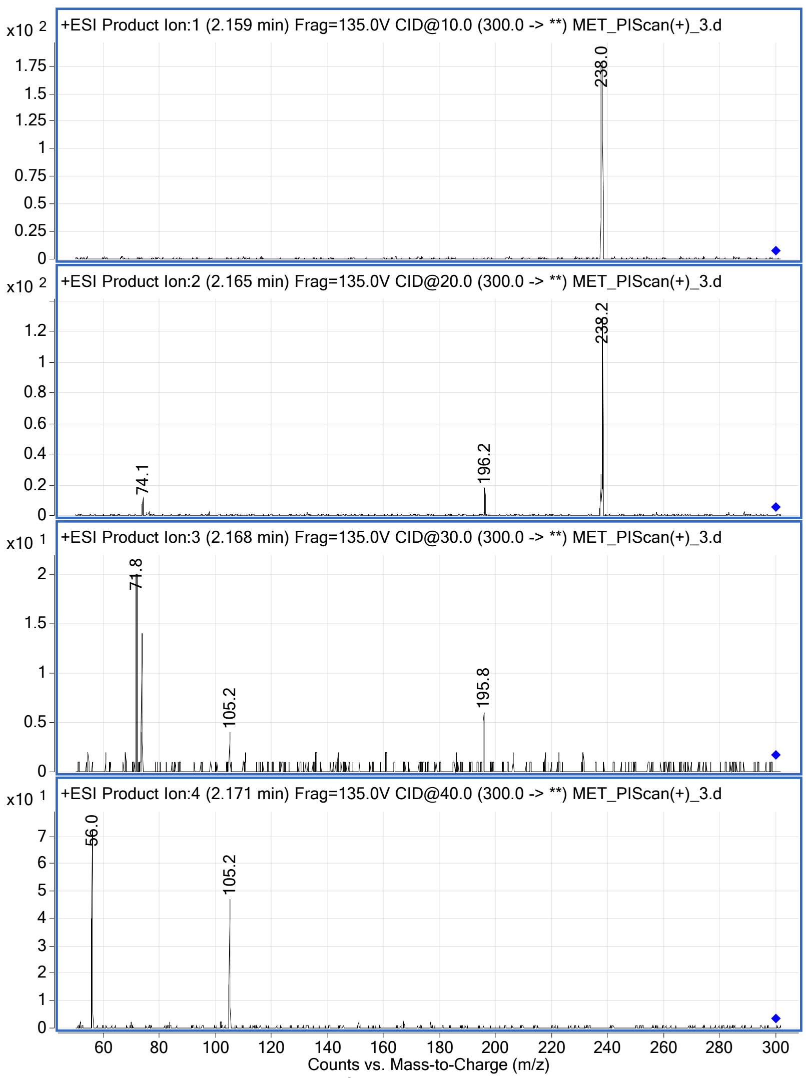

Fig. S16. Positive mode MS^2 spectra of degradation product P7.

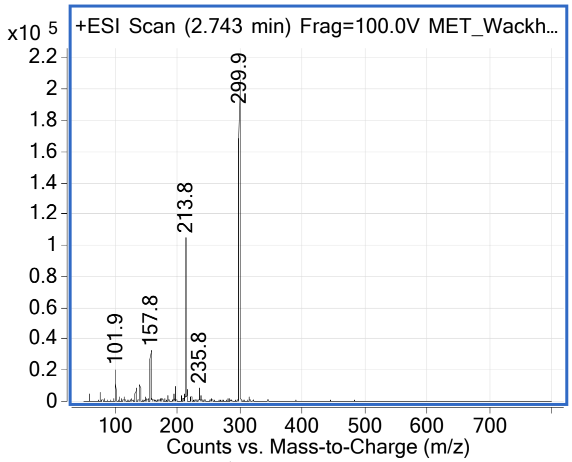

Fig. S17. Positive mode MS^1 spectra of degradation product P8.

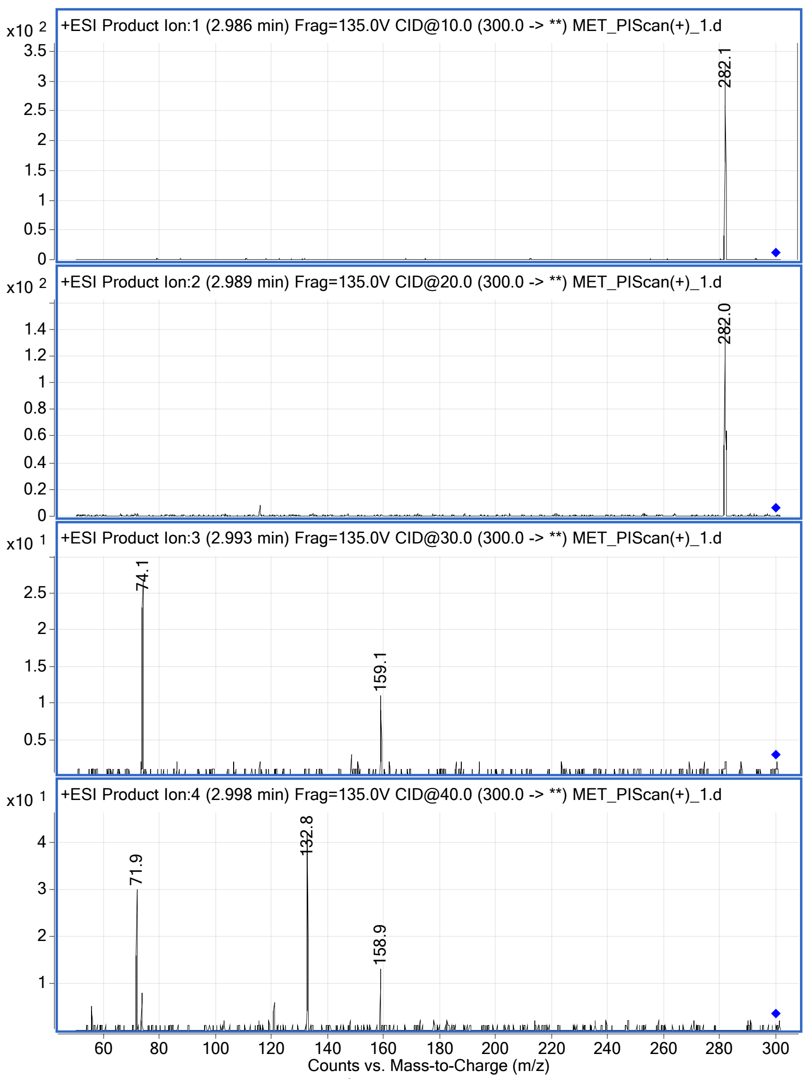

Fig. S18. Positive mode MS^2 spectra of degradation product P8.

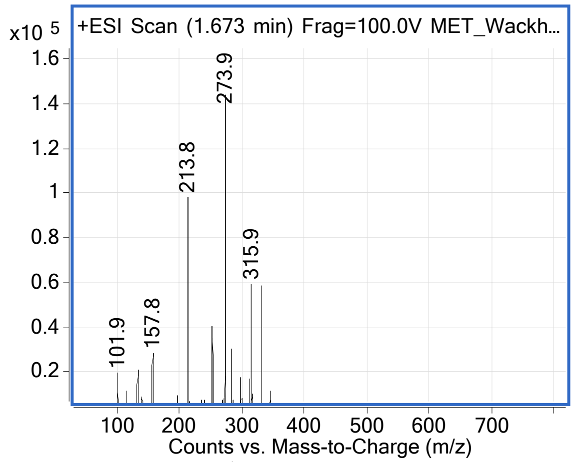

Fig. S19. Positive mode MS^1 spectra of degradation product P9.

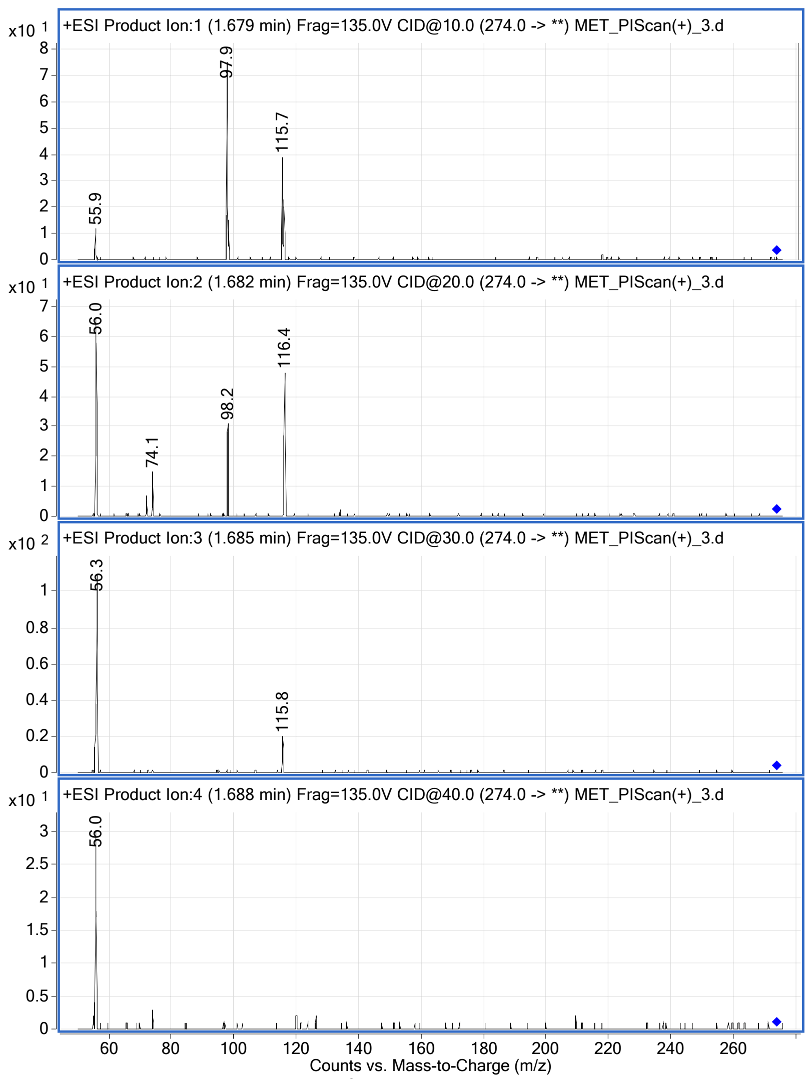

Fig. S20. Positive mode MS^2 spectra of degradation product P9.

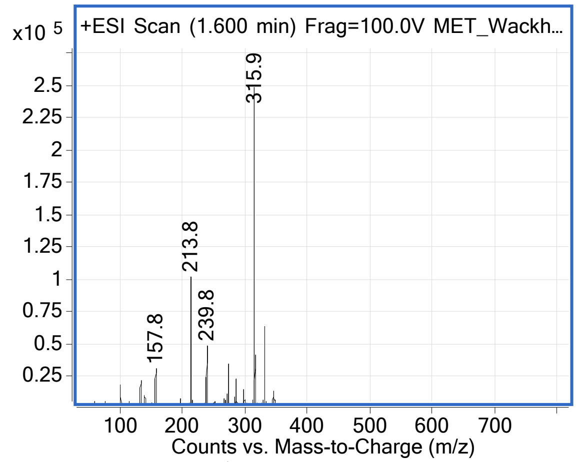

Fig. S21. Positive mode MS^1 spectra of degradation product P10.

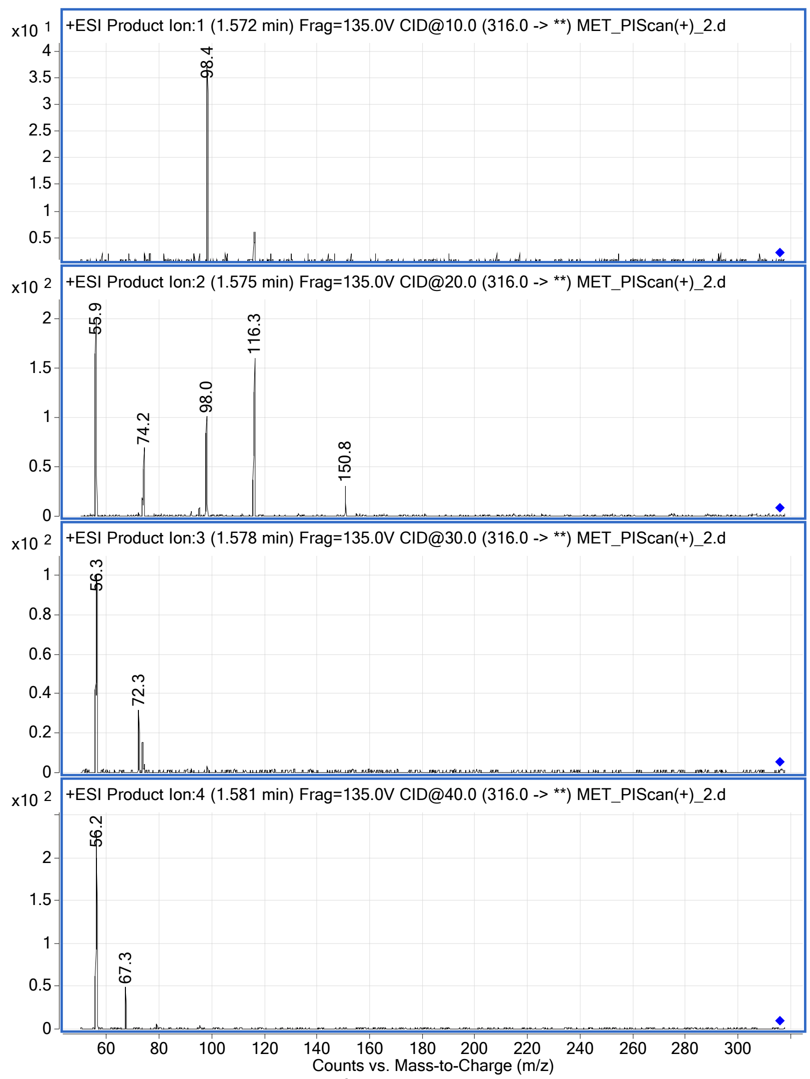

Fig. S22. Positive mode MS^2 spectra of degradation product P10.

Table S1. Proposed structures of intermediates for the photocatalytic degradation of MET in the presence of TiO_2 Wackherr or Degussa P25, with different electron acceptors

Compound	Precursor ion $[M+H]^+$	Molecular formula	Name of compound	V_{col} (V)	Product ions m/z (relative abundance)
MET	268	$C_{15}H_{25}NO_3$	1-[4-(2 methoxyethyl)phenoxy] -3-(propan-2-ylamino)propan-2-ol	10 20 30 40	226(9), 191(76), 176(13), 159(62), 147(11), 133(56), 121(75), 116(100), 98(45), 74(54), 72(62), 56(20) 191(29), 159(59), 148(11), 133(78), 121(91), 116(68), 105(20), 98(43), 74(86), 72(100), 58(16), 56(87) 133(57), 121(42), 116(23), 105(44), 103(21), 74(59), 72(40), 56(100), 133(28), 121(18), 105(20), 103(47), 91(48), 79(26), 77(47), 74(14), 56(100)
P1	134	$C_6H_{15}NO_2$	3-(propan-2-ylamino)propane-1,2-diol	10 20 30 40	134(35), 116(28), 92(51), 74(100), 72(32), 56(46), 74(26), 72(9), 56(100), 56(100) 56(100)
P2*	254	$C_{13}H_{19}NO_4$	Hydroxy derivative 4-[2-hydroxy-3-(propan- 2-ylamino)propoxy]benzaldehyde	10 20 30 40	212(100), 177(24), 133(14), 105(4), 72(8), 56(27) 177(34), 133(38), 105(70), 74(17), 72(28), 56(100) 121(9), 105(19), 79(16), 74(10), 56(100) 121(30), 79(28), 77(24), 65(100), 56(42)
P3	254	$C_{14}H_{23}NO_3$	1-[4-(1-hydroxyethyl)phenoxy]-3-(propan-2-ylamino)propan-2-ol	10 20 30 40	177(100), 116(55), 74(63) 177(8), 159(100), 131(74), 116(8), 72(42), 56(5) 131(100), 105(39), 57(39) 91(59), 56(100)
P4a	282	$C_{15}H_{23}NO_4$	methyl {4-[2-hydroxy-3-(propan-2-ylamino)propoxy]phenyl}acetate; or 1-{4-[2-hydroxy-3-(propan-2-ylamino)propoxy]phenyl}-2-methoxyethanone	composite	240(9), 205(40), 159(20), 149(11), 145(9), 133(100), 116(29), 91(7), 74(8), 56(44)
P4b	282	$C_{15}H_{23}NO_4$	methyl {4-[2-hydroxy-3-(propan-2-ylamino)propoxy]phenyl}acetate; or 1-{4-[2-hydroxy-3-(propan-2-ylamino)propoxy]phenyl}-2-methoxyethanone	composite	240(56), 205(9), 159(74), 145(73), 133(84), 116(45), 103(47), 74(65), 56(100)
P5	282	$C_{15}H_{23}NO_4$	2-hydroxy-3-[4-(2-methoxyethyl)phenoxy]-*N*-(propan-2-yl)propanamide	composite	205 (5), 177(19), 159(64), 145(25), 121(20), 103(20), 98(16), 91(40), 74(64), 72(25), 58(26), 56(100)
P6	282	$C_{15}H_{23}NO_4$	4-(2-methoxyethyl)phenyl 2-hydroxy-3-(propan-2-ylamino)propanoate	composite	264(18), 205(6), 159(53), 145 (16), 133(15) 121(17), 103(13), 116(33), 98(20), 91(33), 74(33), 72(22), 56(100)
P7	300	$C_{15}H_{25}NO_5$	1-{4-[2-hydroxy-3-(propan-2-ylamino)propoxy]phenyl}-2-methoxyethane-1,2-diol	10 20 30 40	238(100) 238(100), 196(12), 74(7) 196(30), 105(20), 74(70), 72(100) 105(65), 56(100)
P8**	300	$C_{15}H_{25}NO_5$	Dihydroxy derivate 1-[4-(2 methoxyethyl)phenoxy] -3-(propan-2-ylamino)propan-2-ol	10 20 30 40	282(100) 282(100), 116(14) 159(32), 74(100) 159(21), 133(100), 74(19), 72(30), 56(17)
P9***	274	$C_{12}H_{19}NO_6$	Trihydroxy derivate 1-amino-3-[4-(2-methoxyethyl)phenoxy]propan-2-ol	10 20 30 40	116(69), 98(100), 56(13) 116(73), 98(47), 74(23), 56(100) 116(18), 56(100) 56(100)
P10****	316	$C_{15}H_{25}NO_6$	Trihydroxy derivate 1-[4-(2-methoxyethyl)phenoxy] -3-(propan-2-ylamino)propan-2-ol	10 20 30 40	116(32), 98(100) 151(17), 116(80), 98(50), 74(43), 56(100) 74(15), 72(32), 56(100) 67(21), 56(100)

P1, P3–P7 were identified in all cases.
P2* was identified, in all cases, only with TiO_2 Wackherr
P8** was identified only with TiO_2 Wackherr/O_2/H_2O_2
P9*** was identified in all cases except TiO_2 Wackherr/O_2
P10 **** was identified in all cases except TiO_2 Wackherr/O_2 and Degussa P25/O_2/$KBrO_3$