Supporting Information

Mechanistic explanation and influence of molecular structure on chemical degradation and toxicity reduction by hydroxyl radicals

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Table S1 Kinetic parameters for Fenton oxidation of ACT, BPA, and TC at ferrous ion concentration of 0.5 mM and varying concentrations of H_2O_2.

| Compound	H_2O_2 concentration (mM)	C_0	C_{equil}	k (min^{-1})	R^2
	0.1	50.01	34.84	1.730	0.9990
ACT	0.3	49.74	21.05	1.688	0.9937
	0.5	49.87	8.42	2.464	0.9977
	0.1	49.99	35.48	2.887	0.9998
BPA	0.3	49.71	24.74	1.612	0.9877
	0.5	50.05	10.46	2.361	0.9997
	0.1	49.98	11.41	3.311	0.9994
TC	0.3	50.00	8.12	3.716	0.9998
	0.5	50.00	4.80	6.500	0.9978

Note: C_0 is the initial concentration of the target compound at 0 min; C_{equil} is the target compound concentration when achieved Fenton equilibrium; k is the first-order kinetic rate constant; R^2 indicates the goodness of kinetic model fitting.

**Table S2** Fukui function value of ACT (H atom data not shown)[1]
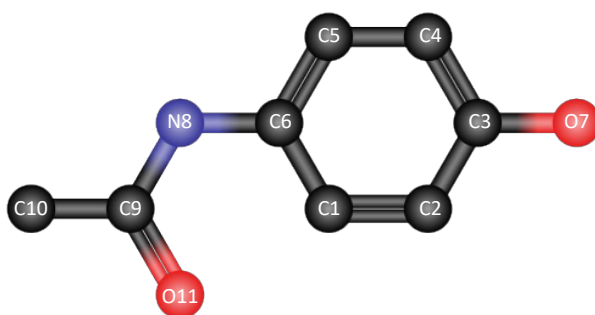
Atom	f^+	f^-	f^0
C1	0.0201	-0.8000	0.3899
C2	0.0658	-0.0096	-0.0282
C3	0.0872	-0.0043	-0.0415
C4	0.0321	-0.0070	-0.0125
C5	-0.0242	0.1226	-0.0492
C6	0.0895	1.0672	-0.5784
O7	0.0772	0.0263	-0.0518
N8	0.0981	-0.3863	0.1441
C9	-0.0145	0.8288	-0.4071
C10	0.0282	-0.3956	0.1837
O11	0.1409	0.2357	-0.1883

Table S3 Fukui function value of BPA (H atom data not shown)[2]
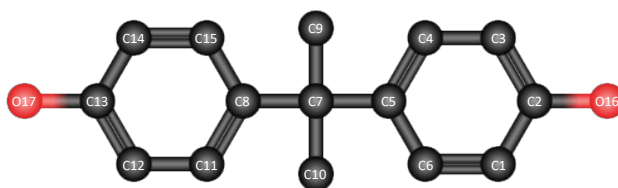
Atom	f^+	f^-	f^0
C1	0.068	0.039	0.053
C2	0.032	0.059	0.045
C3	0.065	0.053	0.059
C4	0.06	0.037	0.048
C5	0.016	0.052	0.034
C6	0.056	0.036	0.046
C7	0.002	0.006	0.004
C8	0.016	0.052	0.034
C9	0.008	0.011	0.01
C10	0.008	0.011	0.01
C11	0.056	0.036	0.046
C12	0.068	0.039	0.053
C13	0.032	0.059	0.045
C14	0.065	0.053	0.059
C15	0.06	0.037	0.048
O16	0.02	0.063	0.041
O17	0.02	0.063	0.041

Table S4 Fukui function value of TC (H atom data not shown)[3]
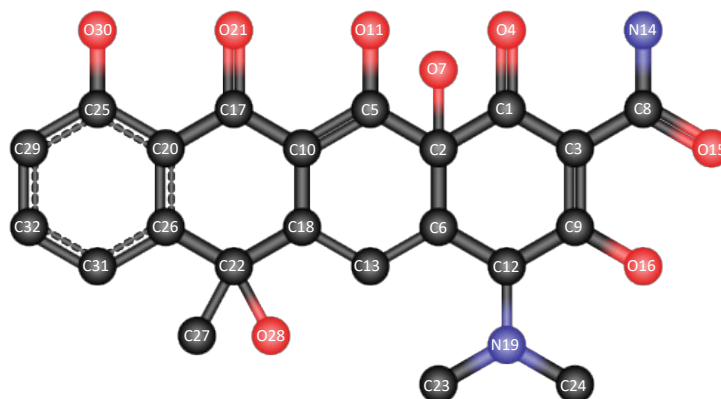
Atom	f^+	f^-	f^0	Atom	f^+	f^-	f^0
C1	-0.0035	0.0062	0.0014	C17	0.1069	0.0028	0.0548
C2	0.0081	0.0036	0.0058	C18	0.0023	0.0019	0.0021
C3	-0.0006	0.0195	0.0094	N19	-0.0005	0.2369	0.1182
O4	0.0150	0.0351	0.0250	C20	0.0122	-0.0027	0.0048
C5	0.0779	-0.0113	0.0333	O21	0.0899	0.0134	0.0517
C6	0.0024	0.0066	0.0045	C22	0.0023	-0.0004	0.0009
O7	0.0200	0.0152	0.0176	C23	0.0048	0.0452	0.0250
C8	0.0077	0.0133	0.0105	C24	0.0031	0.0480	0.0255
C9	-0.0044	0.0072	0.0014	C25	0.0367	0.0079	0.0223
C10	0.0135	0.0009	0.0072	C26	0.0370	-0.0050	0.0160
O11	0.0623	0.0017	0.0320	C27	0.0085	0.0022	0.0053
C12	-0.0018	0.0194	0.0088	O28	0.0099	-0.0154	-0.0028
C13	0.0052	0.0050	0.0051	C29	0.0387	0.0139	0.0263
N14	0.0122	0.0252	0.0187	O30	0.0407	0.0138	0.0272
O15	0.0156	0.0231	0.0194	C31	0.0285	0.0063	0.0174
O16	0.0125	0.0110	0.0118	C32	0.0714	0.0133	0.0424

REFERENCES

(1) Qutob, M.; Hussein, M. A.; Alamry, K. A.; Rafatullah, M. A review on the degradation of acetaminophen by advanced oxidation process: pathway, by-products, biotoxicity, and density functional theory calculation. *RSC Advances* **2022**, *12* (29), 18373-18396, 10.1039/D2RA02469A. DOI: 10.1039/D2RA02469A.

(2) Lee, J.; Eom, S.; Sohn, S.; Kim, T.; Zoh, K.-D. Degradation of bisphenol A, bisphenol S, and bisphenol AF in the UV-LED/chlorine reaction: Effect of pH on the kinetics, transformation products, and degradation pathway. *Chemical Engineering Journal* **2023**, *470*, 144041. DOI: https://doi.org/10.1016/j.cej.2023.144041.

(3) Fang, C.; Wang, S.; Xu, H.; Huang, Q. Degradation of tetracycline by atmospheric-pressure non-thermal plasma: Enhanced performance, degradation mechanism, and toxicity evaluation. *Science of The Total Environment* **2022**, *812*, 152455. DOI: https://doi.org/10.1016/j.scitotenv.2021.152455.