nanomaterials

MDPI

One-Step Synthesized Iron-Carbon Core-Shell Nanoparticles to Activate Persulfate for Effective Degradation of Tetrabromobisphenol A: Performance and Activation Mechanism

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Table S1. The summaries of reported organic pollutants degradation conditions and performances by iron-based activators.

Catalyst	（g/L）	pollutant	(mg/L)	PS/PDS	pH	Reaction Time (min)	Removal efficiency (%)	Reference
Fe@MC	0.2	TBBPA	10	2.0	7.0	10	94.9	This work
MCFe	0.5	2,4,6-TCP	100	2.0	3	180	94.8	[1]
Fe@CN	0.1	BPA	20	0.5	6.8	60	96.0	[2]
Fe/Co@mHS	1	TBBPA	10	20.0	5	6	97.13	[3]
AC@Fe_3O_4	0.4	TC	10	40	3	180	99.8	[4]
Fe0@Fe_3O_4	0.5	DPB	5	1.8	7	180	94.7	[5]

Table S2. The basic information of the actual contaminated water.

pH	Electrical conductivity ($ms \cdot cm^{-1}$)	COD ($mg \cdot L^{-1}$)	TOC ($mg \cdot L^{-1}$)	Turbidity (NTU)
8.22	1.10	202.0	160.1	87

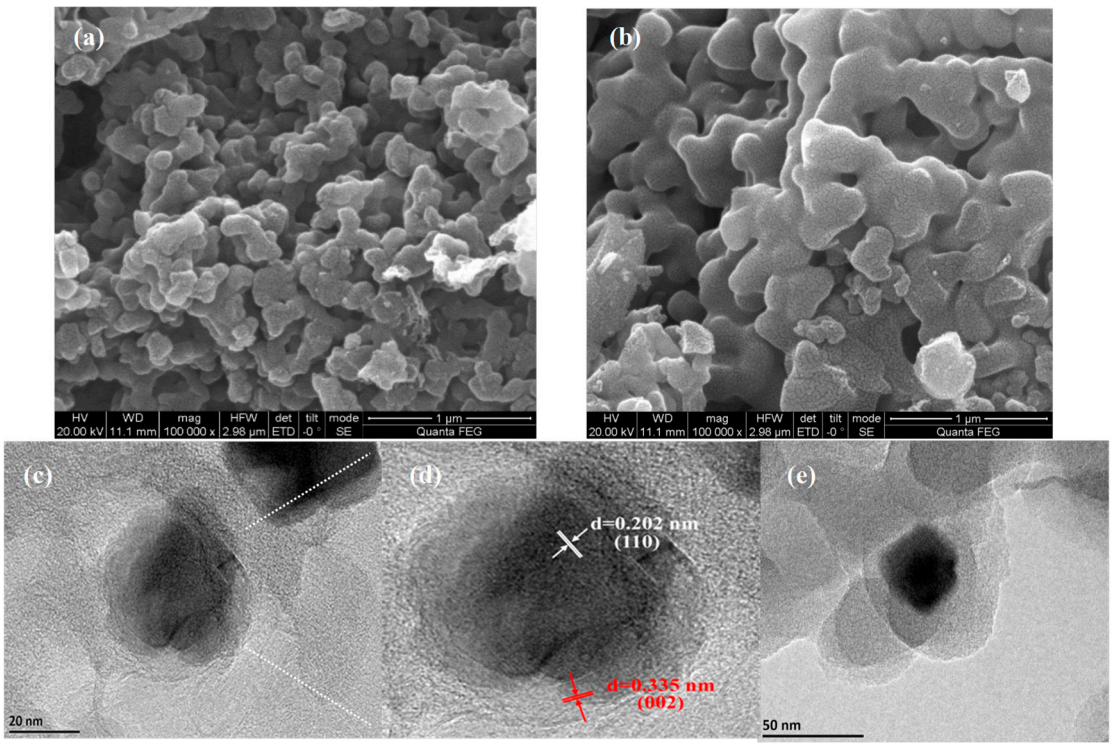


Figure S1. SEM (**a** 800 °C, **b** 1200 °C) and TEM image of (**b,c,d**) Fe@MC.

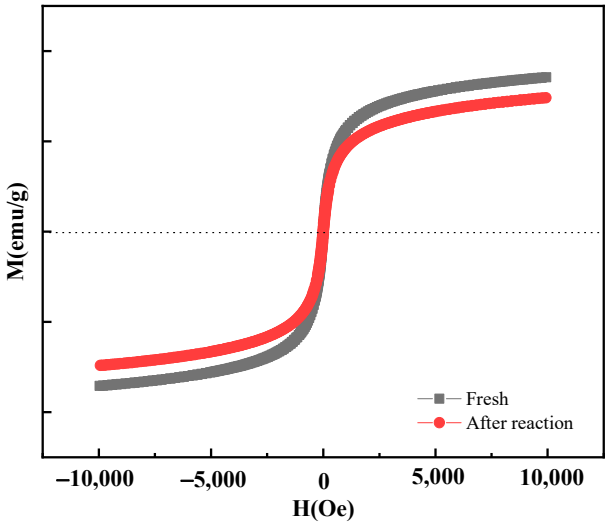


Figure S2. Hysteresis curve image of Fe@MC

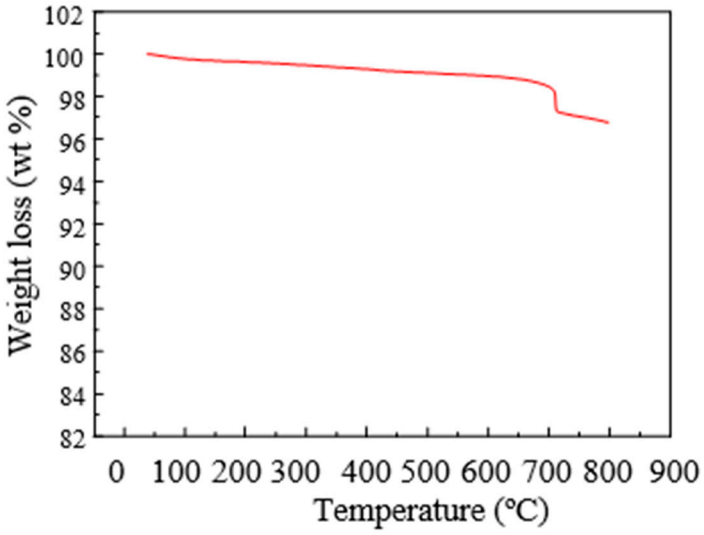


Figure S3. TGA of Fe@MC.

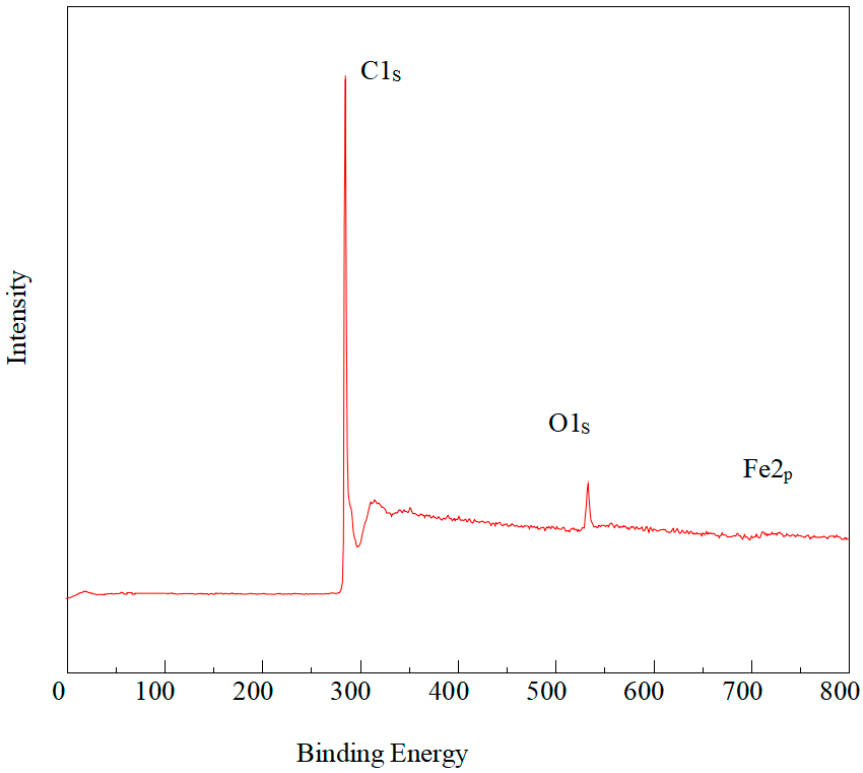
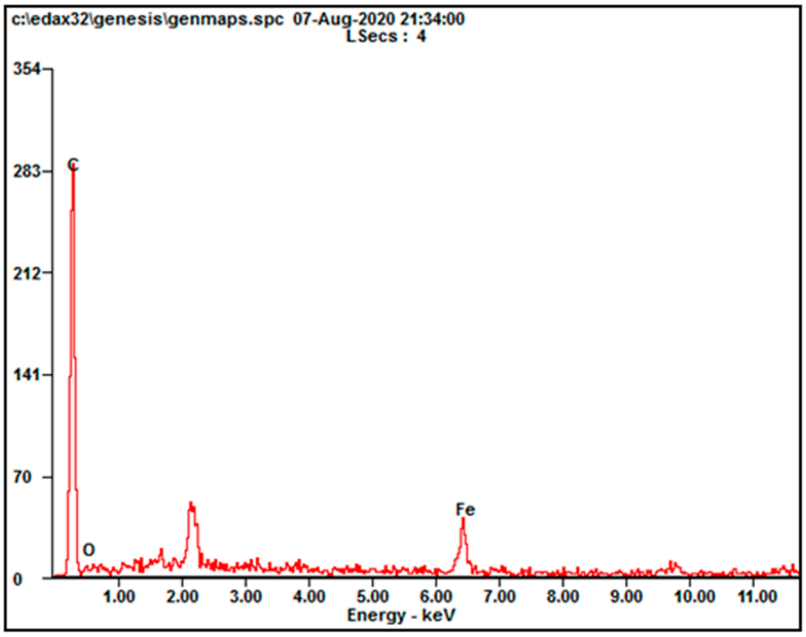


Figure S4. Full XPS spectrum Fe@MC .



	Wt%	At%
CK	88.49	95.77
OK	02.67	02.17
FeK	08.84	02.06
Matrix	Correction	ZAF

Figure S5. The relative content of C, O, Fe analyzed by SEM-EDX.

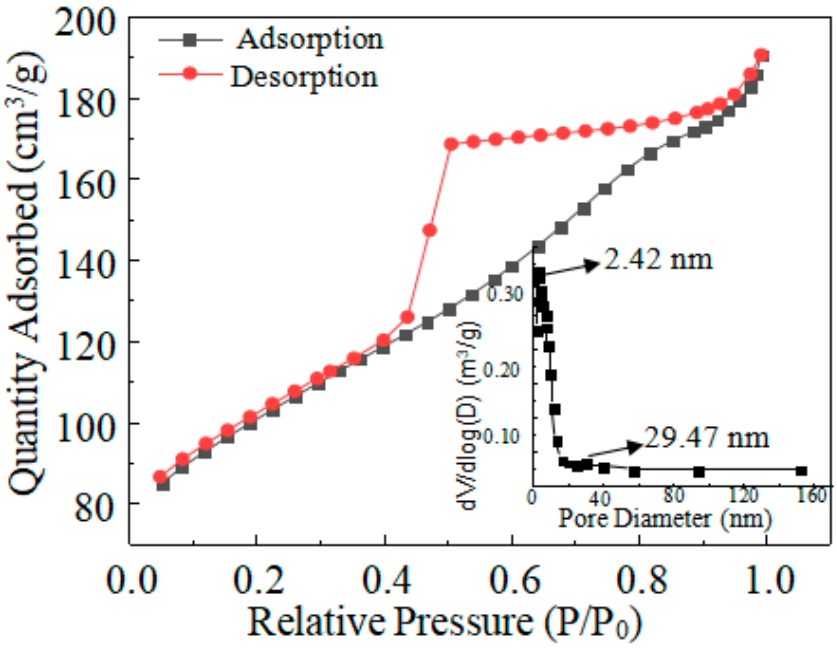


Figure S6. N_2 adsorption-desorption isotherms and pore size distributions of Fe@MC.

Figure S7.

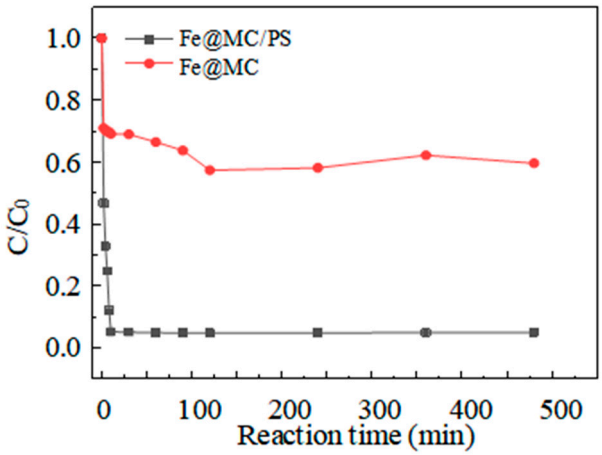


Figure S7. Effect of PS Addition on Removal of TBBPA

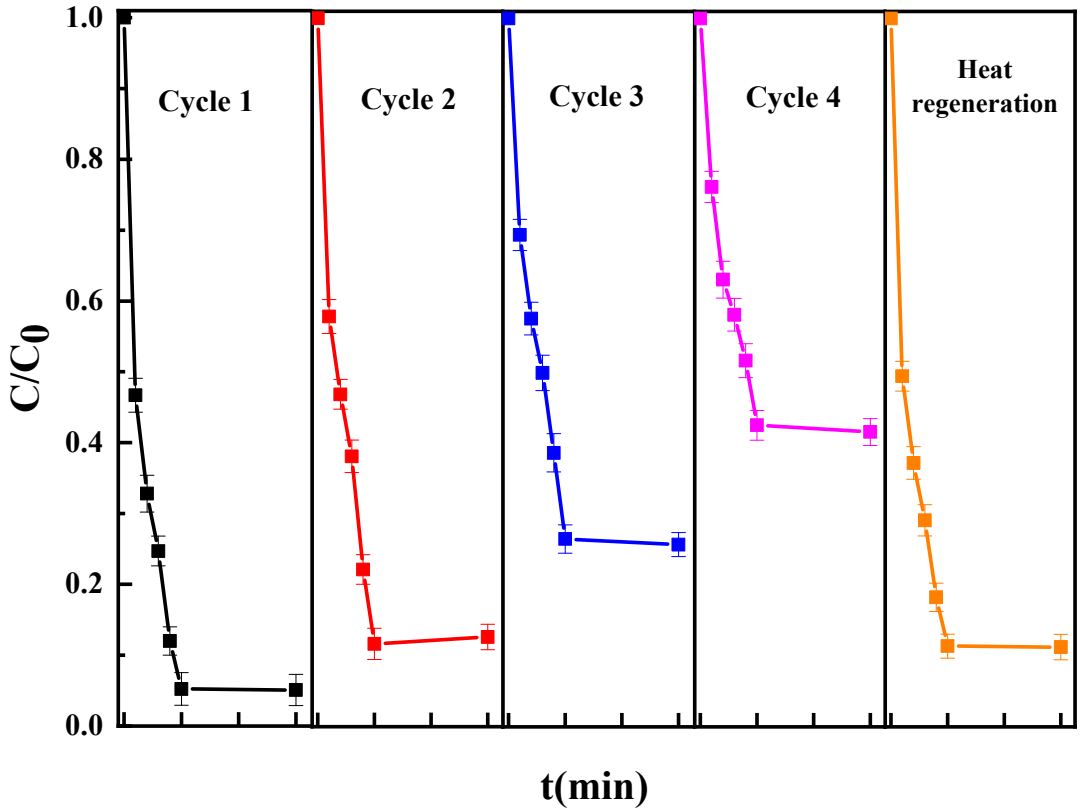


Figure S8. Recyclability and regeneration of Fe@MC

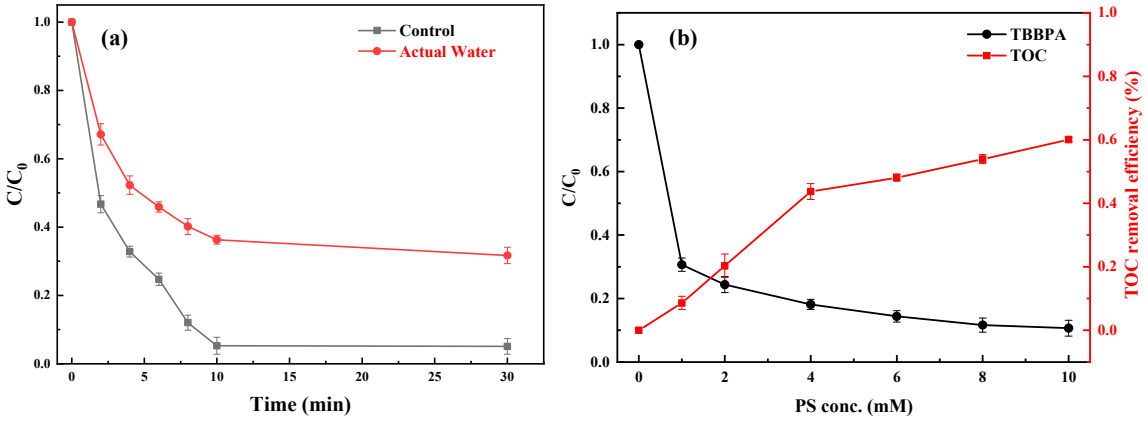


Figure S9. The removal of TBBPA by Fe@MC/PS in actual contaminated water(**a**) and TOC removal removal efficiency with different PS concentration (b).

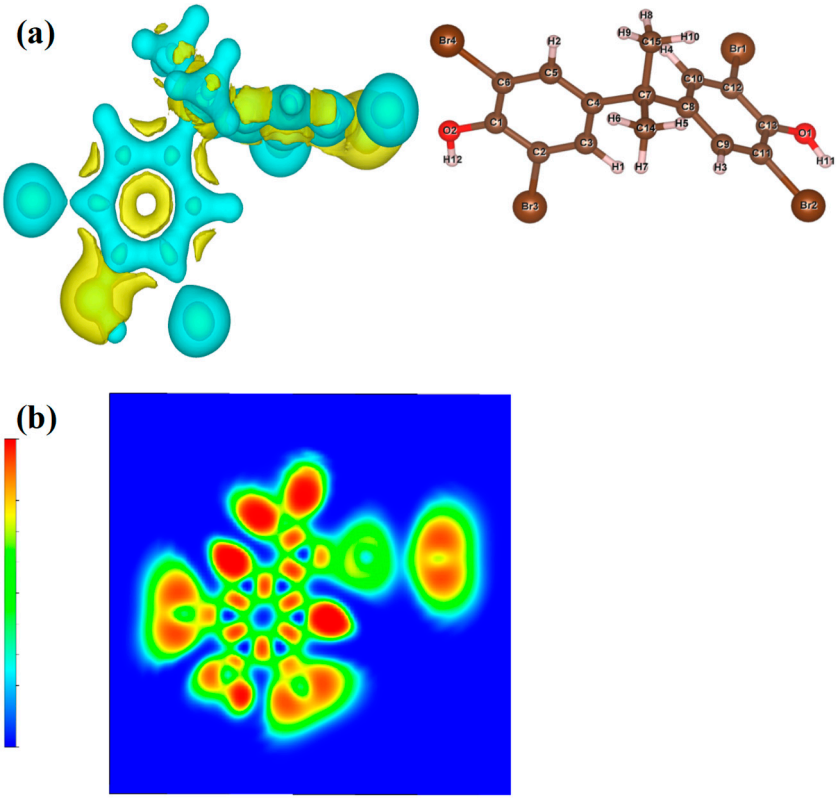
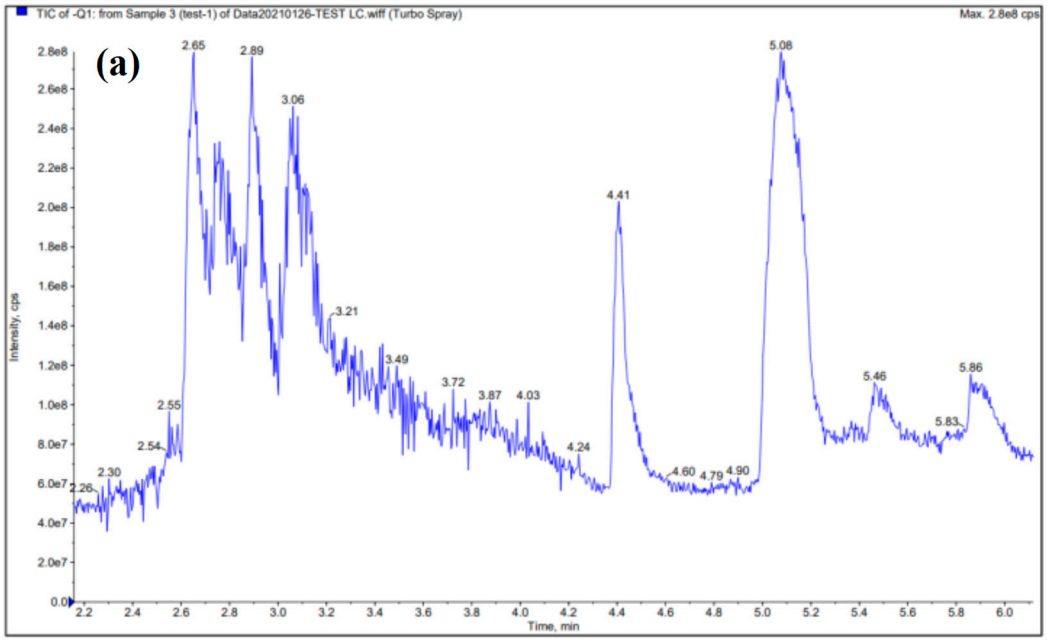
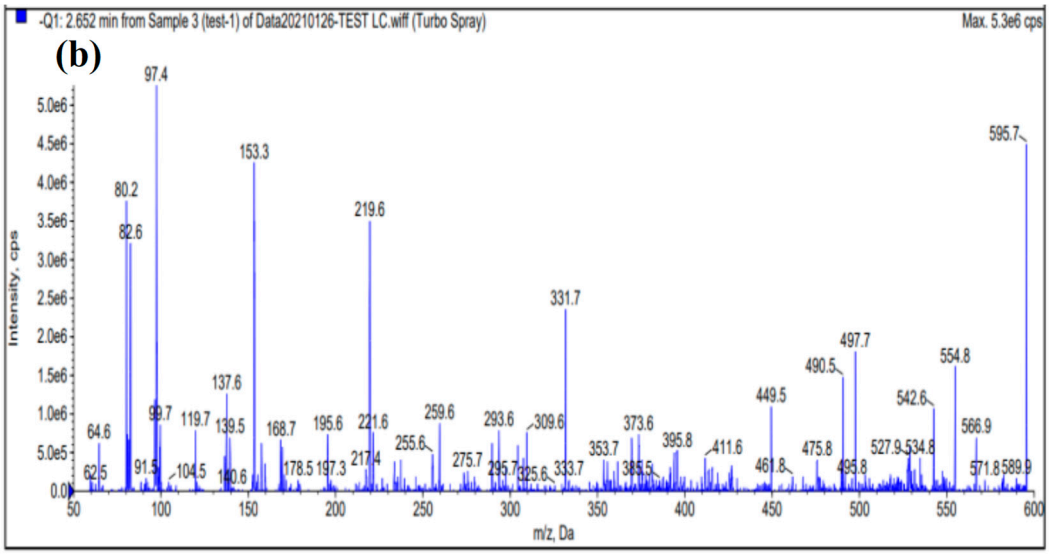
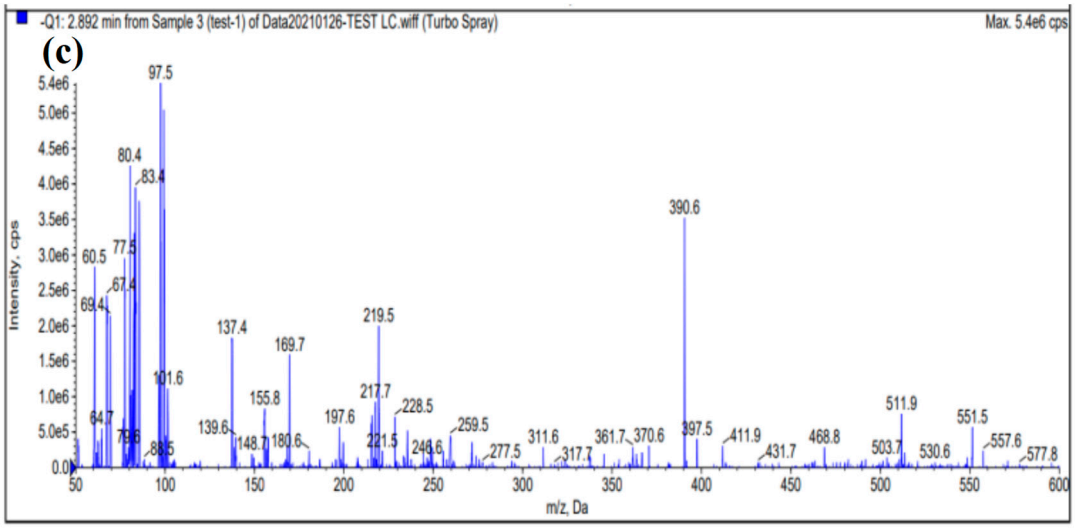


Figure S10. Electron density Laplacian analysis (**a**) and projection map of electron localization function ELF (**b**) of TBBPA.


TIC of -Q1: from Sample 3 (test-1) of Data20210126-TEST LC.wiff (Turbo Spray)
Max. 2.8e8 cps
(a)
Intensity, cps
Time, min


-Q1: 2.652 min from Sample 3 (test-1) of Data20210126-TEST LC.wiff (Turbo Spray)
Max. 5.3e6 cps
(b)
Intensity, cps
m/z, Da


-Q1: 2.892 min from Sample 3 (test-1) of Data20210126-TEST LC.wiff (Turbo Spray)
Max. 5.4e6 cps
(c)
Intensity, cps
m/z, Da

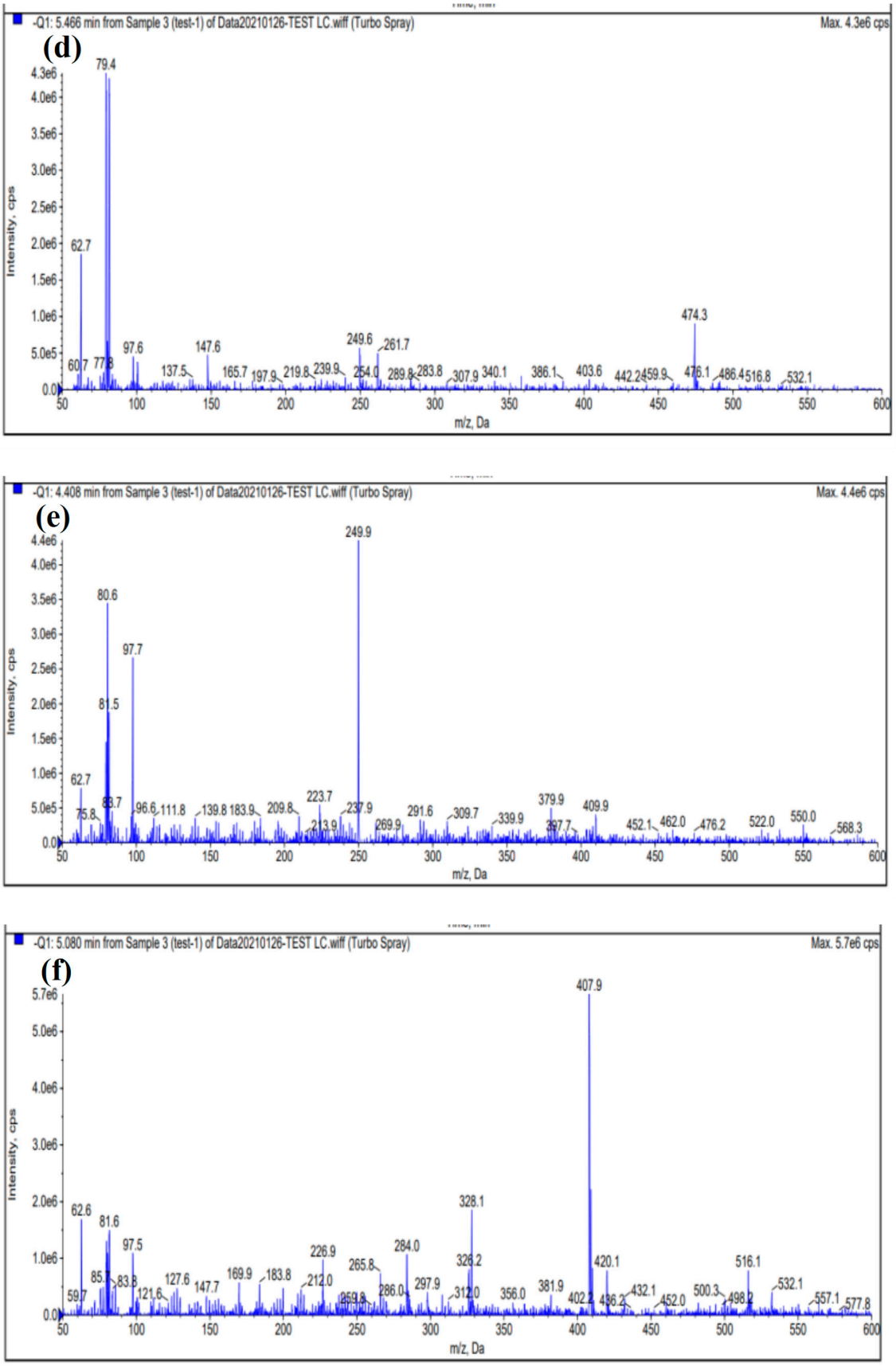


Figure S11. Corresponding mass spectra and structure of degradation products of TBBPA(The total mass spectra of degradation products (a) and each degradation product mass spectra (b,c,d,e,f)).

1. Wu, Y.W.; Chen, X.T.; Han, Y.; Yue, D.T.; Cao, X.D.; Zhao, Y.X.; Qian, X.F. Highly Efficient Utilization of Nano-Fe(0) Embedded in Mesoporous Carbon for Activation of Peroxydisulfate. *Environ. Sci. Technol.* **2019**, *53*, 9081–9090.
2. Liu, L.; Xu, X.; Li, Y.w.; Su, R.D.; Li, Q.; Zhou, W.Z.; Gao, B.Y.; Yue,Q. Y. One-step synthesis of "nuclear-shell" structure iron-carbon nanocomposite as a persulfate activator for bisphenol A degradation. *Chem. Eng. J.* **2020**, *382*, 122780.
3. Xiang, M.H.; Huang, M.F.; Li, H.; Wang, W.B.; Huang, Y.; Lu, Z.; Wang, C.; Si, R.F.; Cao, W. Nanoscale zero-valent iron/cobalt@mesoporous hydrated silica core–shell particles as a highly active heterogeneous Fenton catalyst for the degradation of tetrabromobisphenol A. *Chem. Eng. J.* **2021**, *417*, 129208.
4. Li, H.X.; Wan, J.Q.; Ma, Y.W.; Yan, W. Synthesis of novel core–shell Fe@Fe_3O_4 as heterogeneous activator of persulfate for oxidation of dibutyl phthalate under neutral conditions. *Chem. Eng. J.* **2016**, *301*, 315-324.
5. Jonidi, J.A.; Kakavandi, B.; Jaafarzadeh, N.; Rezaei, K,R.; Ahmadi, M.; Akbar, B,A. Fenton-like catalytic oxidation of tetracycline by AC@Fe_3O_4 as a heterogeneous persulfate activator: Adsorption and degradation studies. *Ind. Eng. Chem.* **2017**, *45*, 323-333.