Supplementary Material

Multi-heteroatom-doping promotes molecular oxygen activation on polymeric carbon nitride for simultaneous generation of H_2O_2 and degradation of oxcarbazepine

Derui Chen[a], Bingling Yao[a], Xinyu Zhi[a], Chang Tian[a], Minghao Chen[a], Siyi Cao[a], Xinyu Feng[a], Huinan Che[a]*, Kan Zhang[b]*, Yanhui Ao[a]

[a]*Key Laboratory of Integrated Regulation and Resource Development on Shallow Lakes, Ministry of Education, College of Environment, Hohai University, No.1, Xikang road, Nanjing, 210098, China*

[b]*Key Laboratory of Advanced Display Material and Devices, School of Materials Science and Engineering, Nanjing University of Science and Technology, 210094 Nanjing, China*

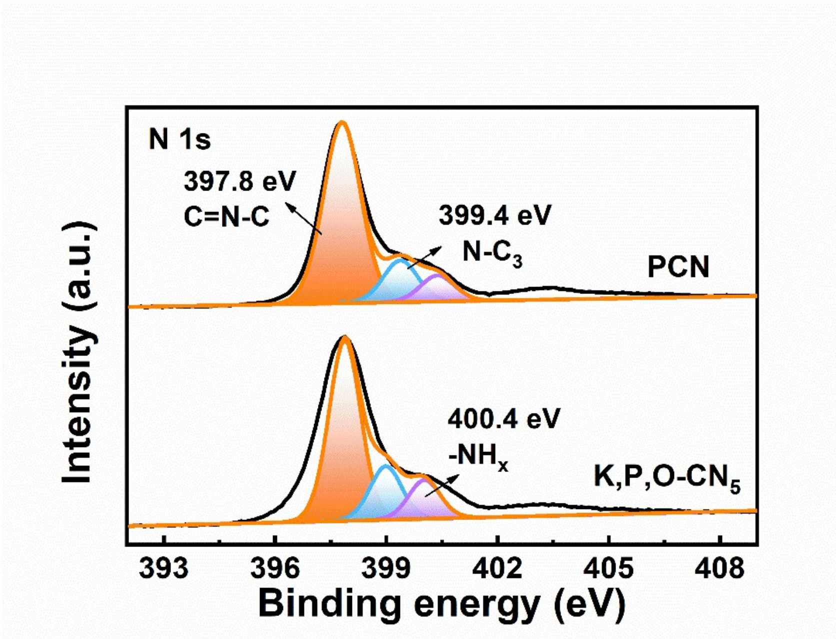


Fig. S1. The N 1s high-resolution XPS spectra of PCN and K, P, O-CN_5.

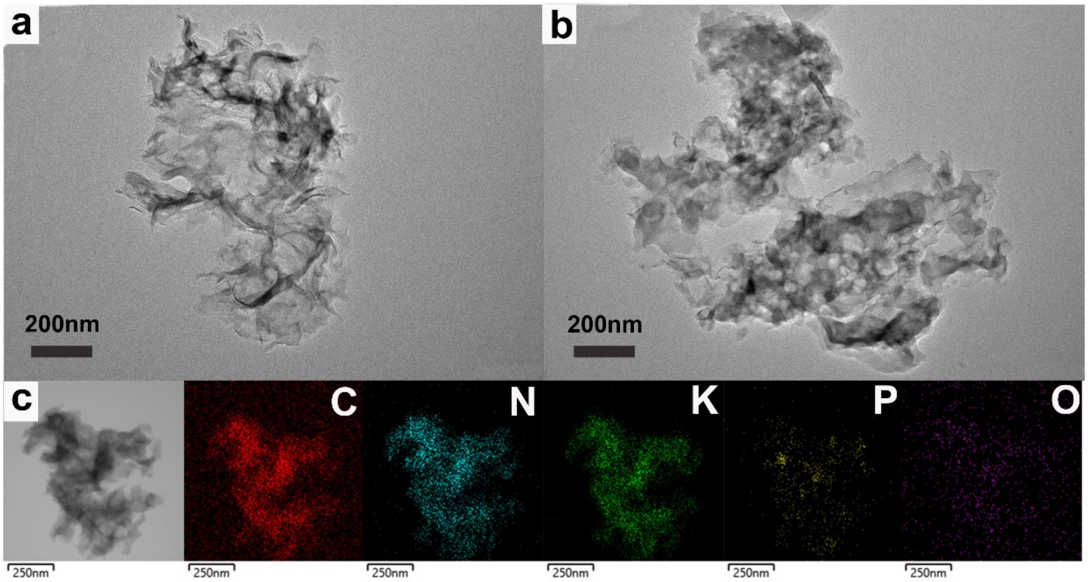


Fig. S2. TEM images of (a) PCN, (b) K, P, O-CN_5, (c) The elements mapping images of K, P, O-CN_5.

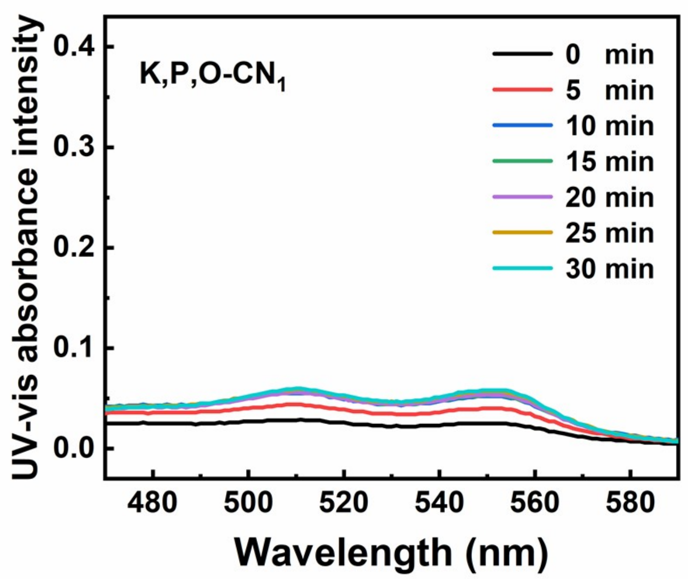


Fig. S3. UV–vis absorption spectra of H_2O_2 produced with IPA in photocatalytic stage of K, P, O-CN_1 at different times.

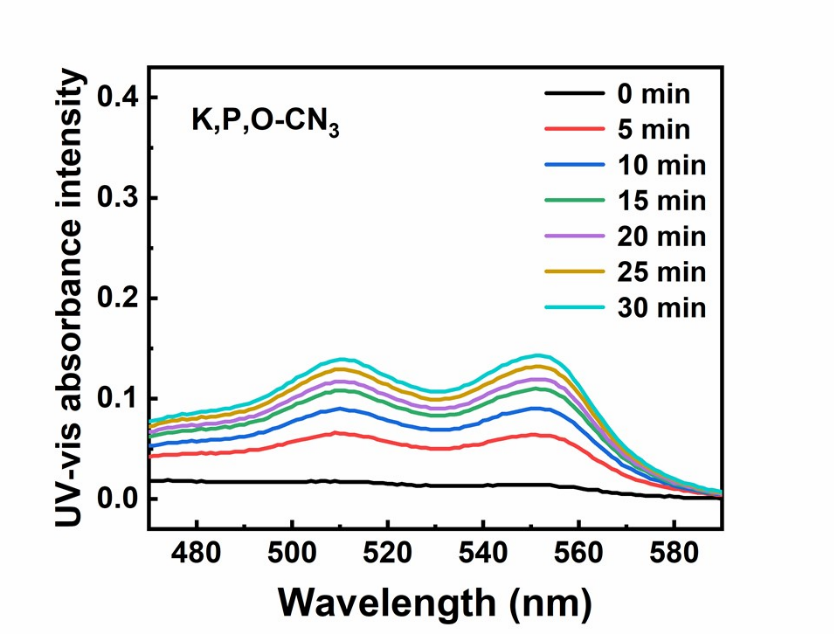


Fig. S4. UV–vis absorption spectra of H_2O_2 produced with IPA in photocatalytic stage of K, P, O-CN_3 at different times.

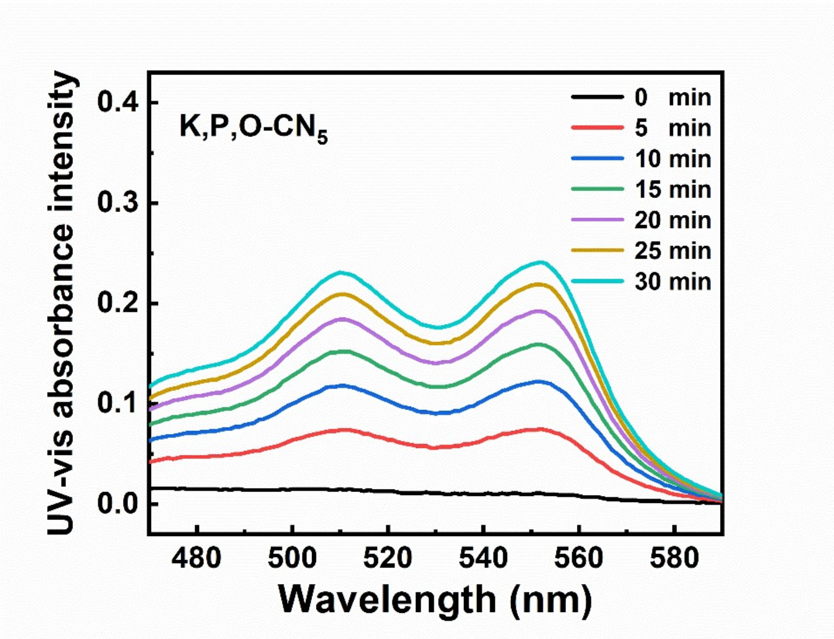


Fig. S5. UV–vis absorption spectra of H_2O_2 produced with IPA in photocatalytic stage of K, P, O-CN_5 at different times.

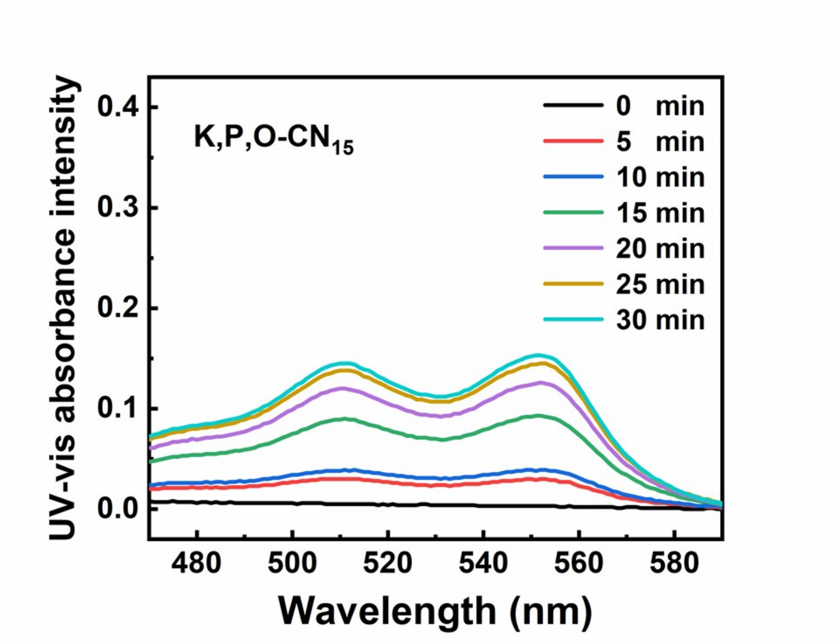


Fig. S6. UV–vis absorption spectra of H_2O_2 produced with IPA in photocatalytic stage of K, P, O-CN_{15} at different times.

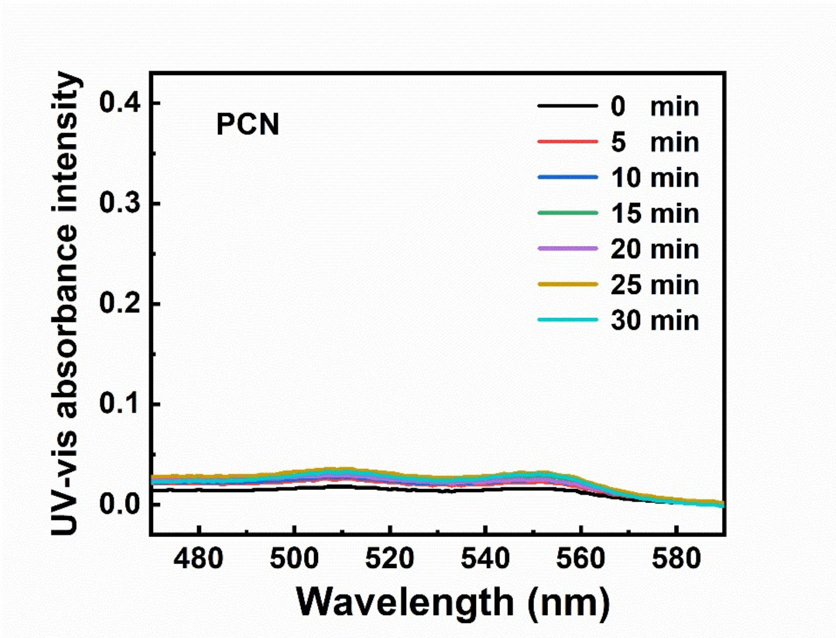


Fig. S7. UV–vis absorption spectra of H_2O_2 produced with IPA in photocatalytic stage of PCN at different times.

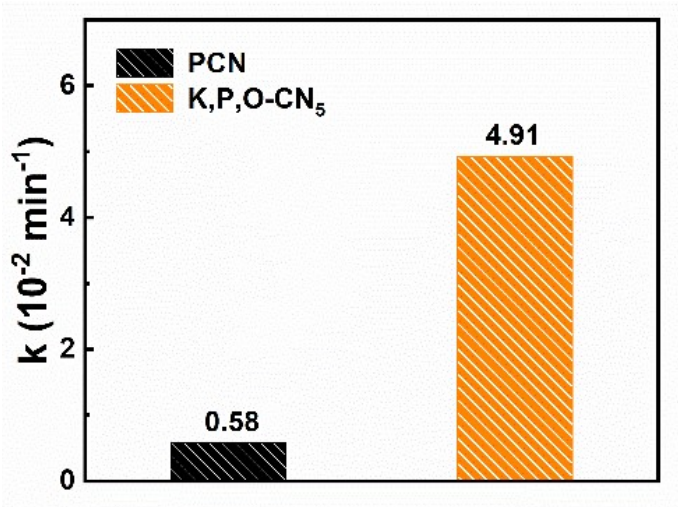


Fig. S8. The first-order reaction kinetic constants of OXC degradation on PCN as well as K, P, O-CN_5.

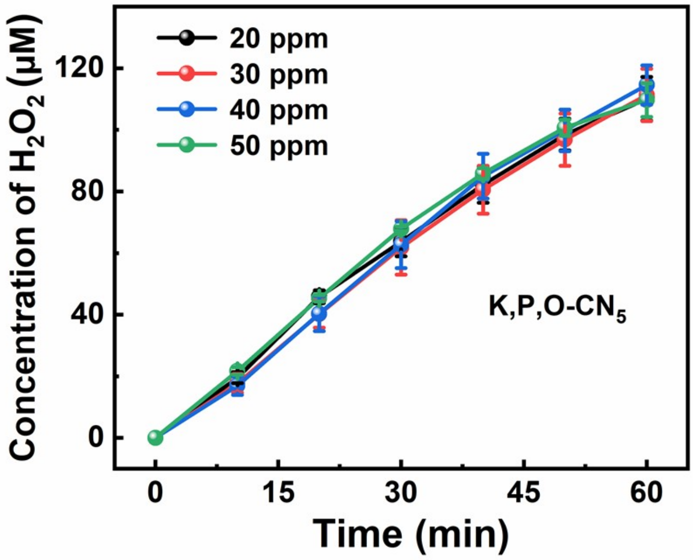


Fig. S9. Photocatalytic H_2O_2 production of K, P, O-CN_5 in the presence of oxcarbazepine with different concentrations.

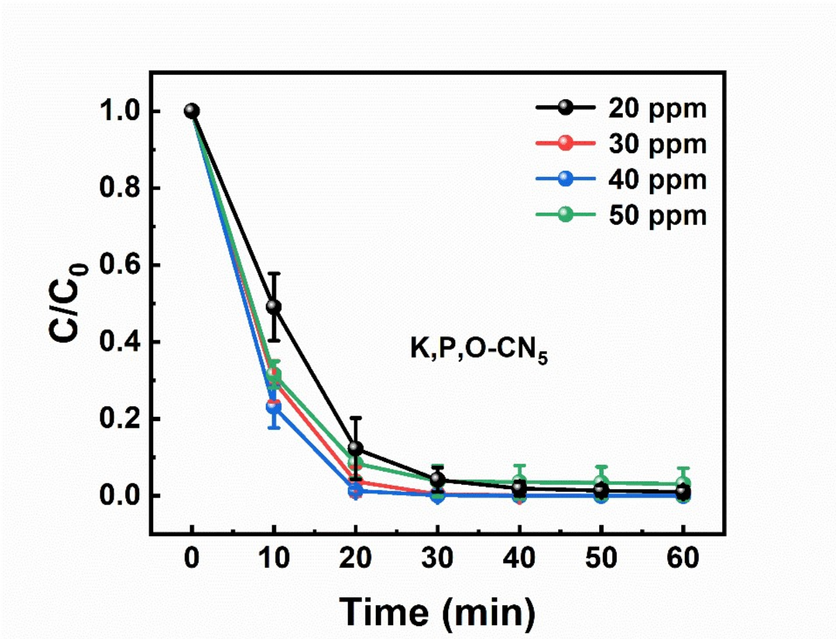


Fig. S10. Degradation efficiency of K, O, P-CN_5 in oxcarbazepine solutions of different concentrations.

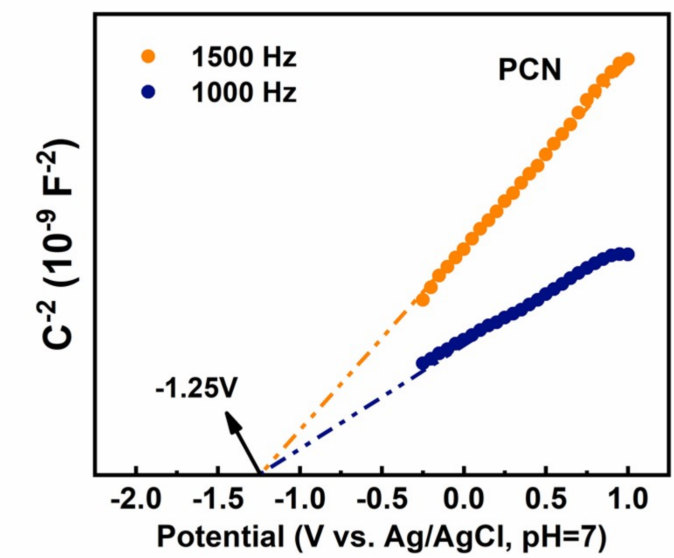


Fig. S11. Mott-Schottky plots collected at different frequencies of PCN.

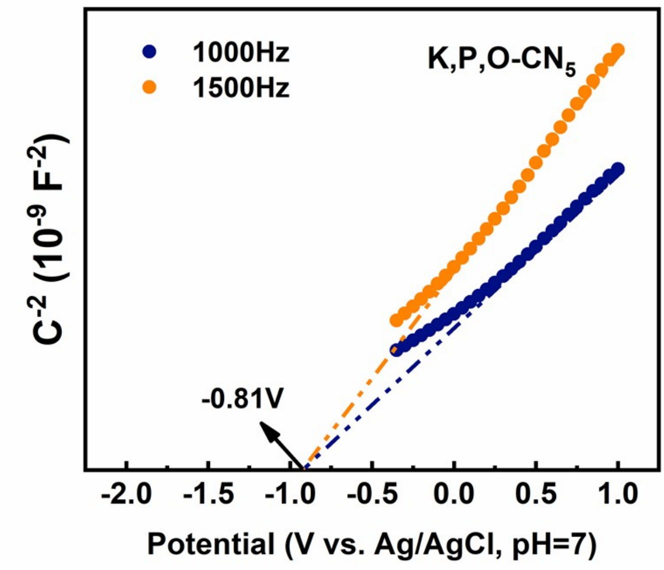


Fig. S12. Mott-Schottky plots collected at different frequencies of K, P, O-CN_5.

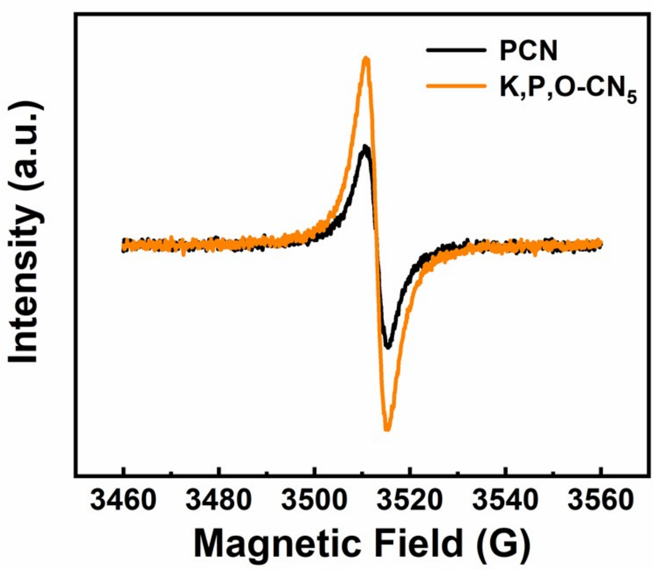
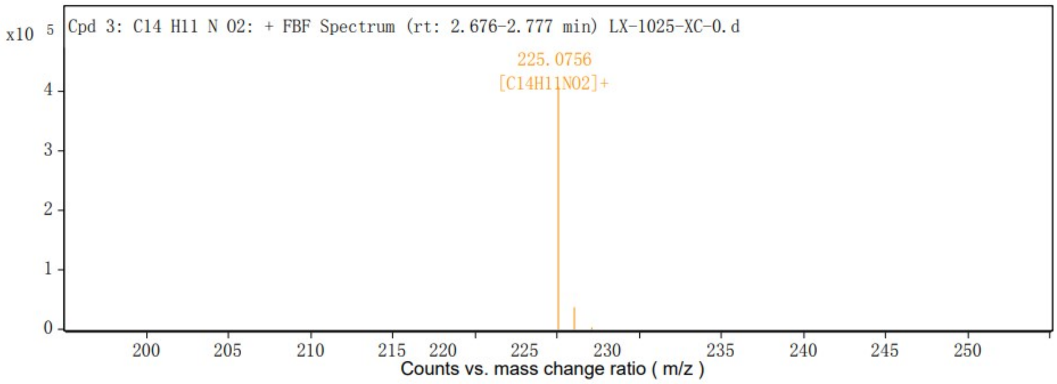
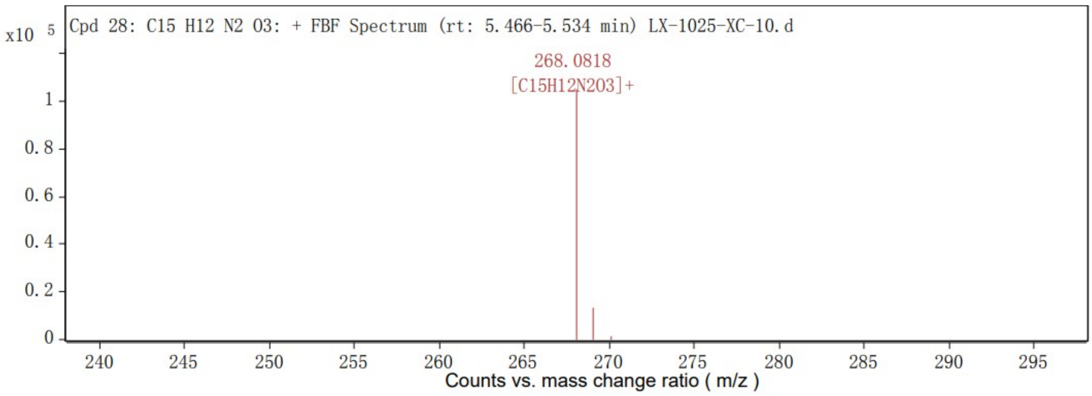


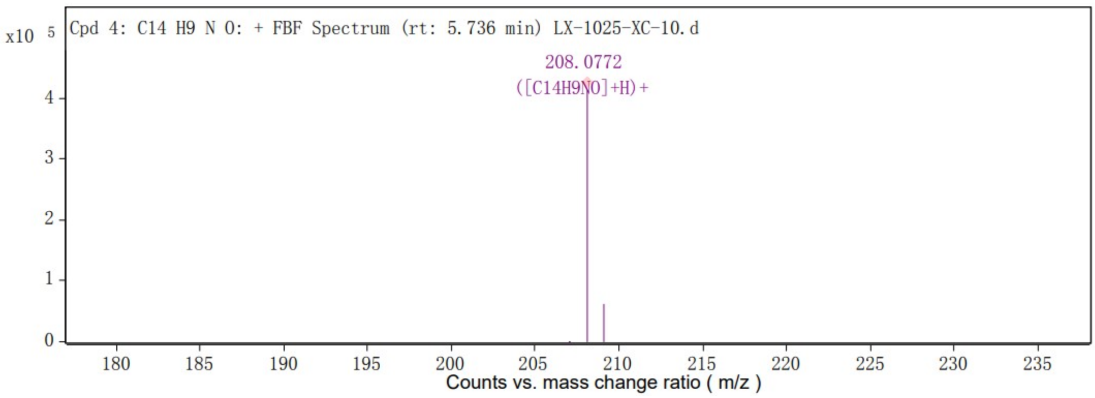
Fig. S13. EPR signals of PCN and K, P, O-CN_5.



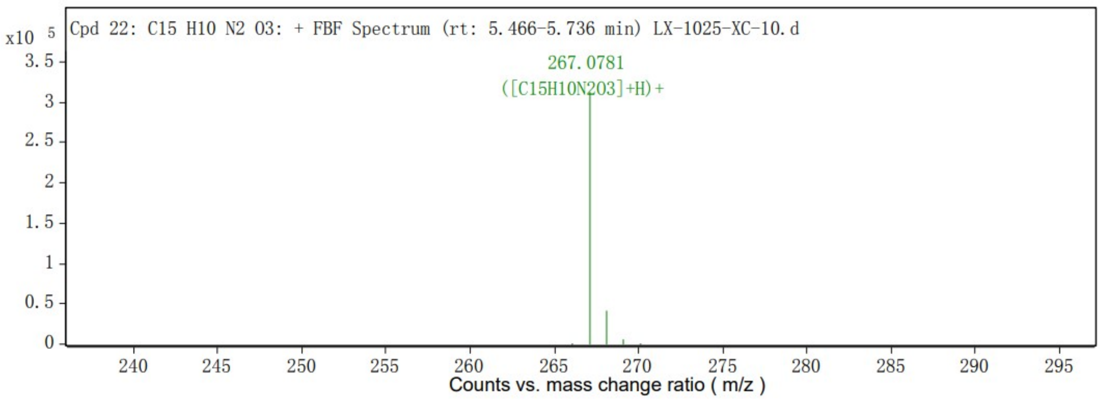
Cpd 3: C14 H11 N O2: + FBF Spectrum (rt: 2.676-2.777 min) LX-1025-XC-0.d
225.0756
[C14H11NO2]+
Counts vs. mass change ratio (m/z)



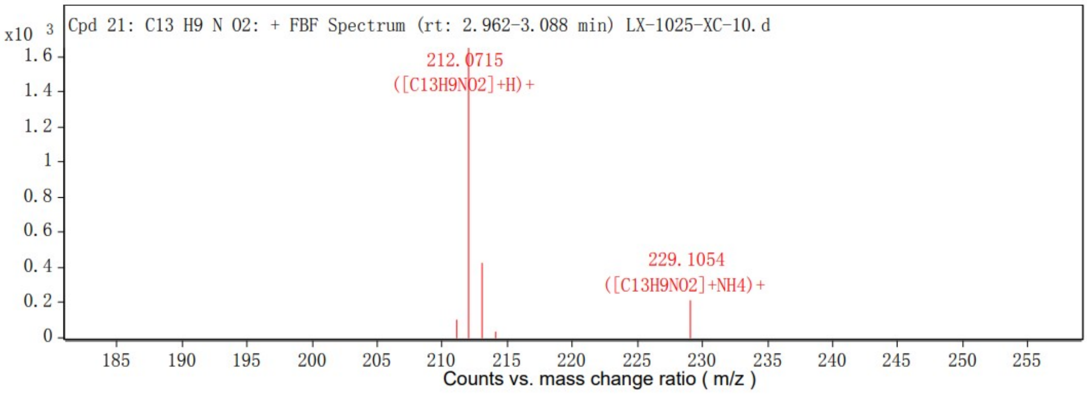
Cpd 28: C15 H12 N2 O3: + FBF Spectrum (rt: 5.466-5.534 min) LX-1025-XC-10.d
268.0818
[C15H12N2O3]+
Counts vs. mass change ratio (m/z)



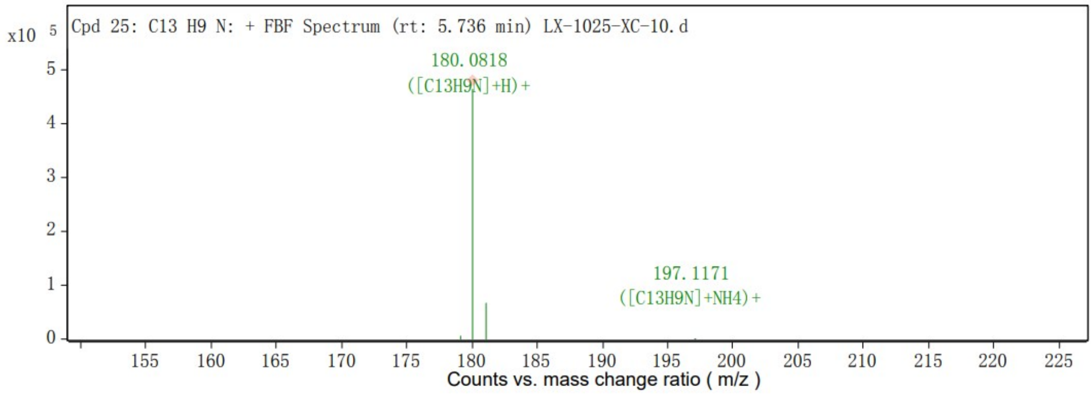
Cpd 4: C14 H9 N O: + FBF Spectrum (rt: 5.736 min) LX-1025-XC-10.d
208.0772
([C14H9NO]+H)+
Counts vs. mass change ratio (m/z)



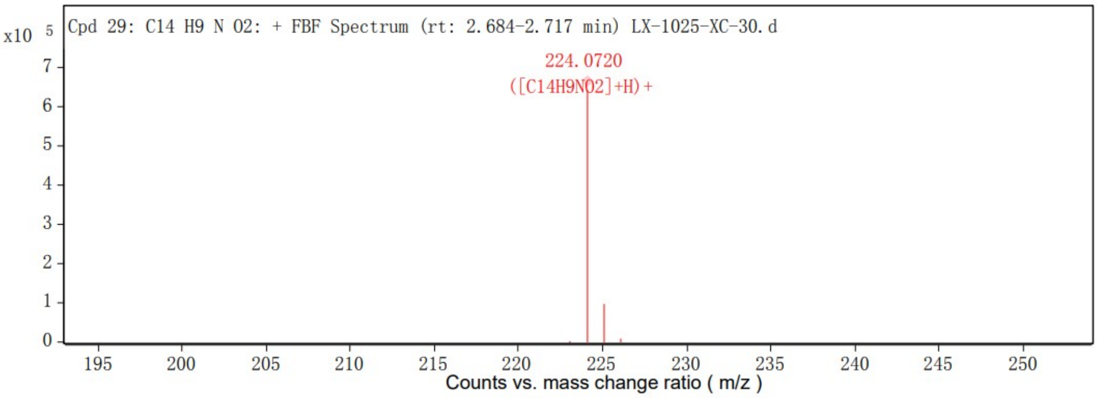
Cpd 22: C15 H10 N2 O3: + FBF Spectrum (rt: 5.466-5.736 min) LX-1025-XC-10.d
267.0781
([C15H10N2O3]+H)+
Counts vs. mass change ratio (m/z)



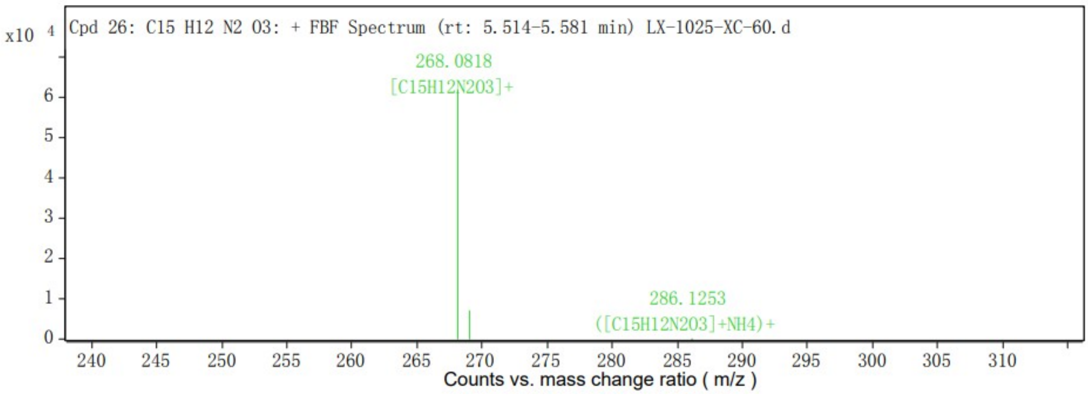
Cpd 21: C13 H9 N O2: + FBF Spectrum (rt: 2.962-3.088 min) LX-1025-XC-10.d
x10 3
212.0715
([C13H9NO2]+H)+
229.1054
([C13H9NO2]+NH4)+
Counts vs. mass change ratio (m/z)



Cpd 25: C13 H9 N: + FBF Spectrum (rt: 5.736 min) LX-1025-XC-10.d
x10 5
180.0818
([C13H9N]+H)+
197.1171
([C13H9N]+NH4)+
Counts vs. mass change ratio (m/z)



Cpd 29: C14 H9 N O2: + FBF Spectrum (rt: 2.684-2.717 min) LX-1025-XC-30.d
x10 5
224.0720
([C14H9NO2]+H)+
Counts vs. mass change ratio (m/z)



Cpd 26: C15 H12 N2 O3: + FBF Spectrum (rt: 5.514-5.581 min) LX-1025-XC-60.d
x10 4
268.0818
[C15H12N2O3]+
286.1253
([C15H12N2O3]+NH4)+
Counts vs. mass change ratio (m/z)

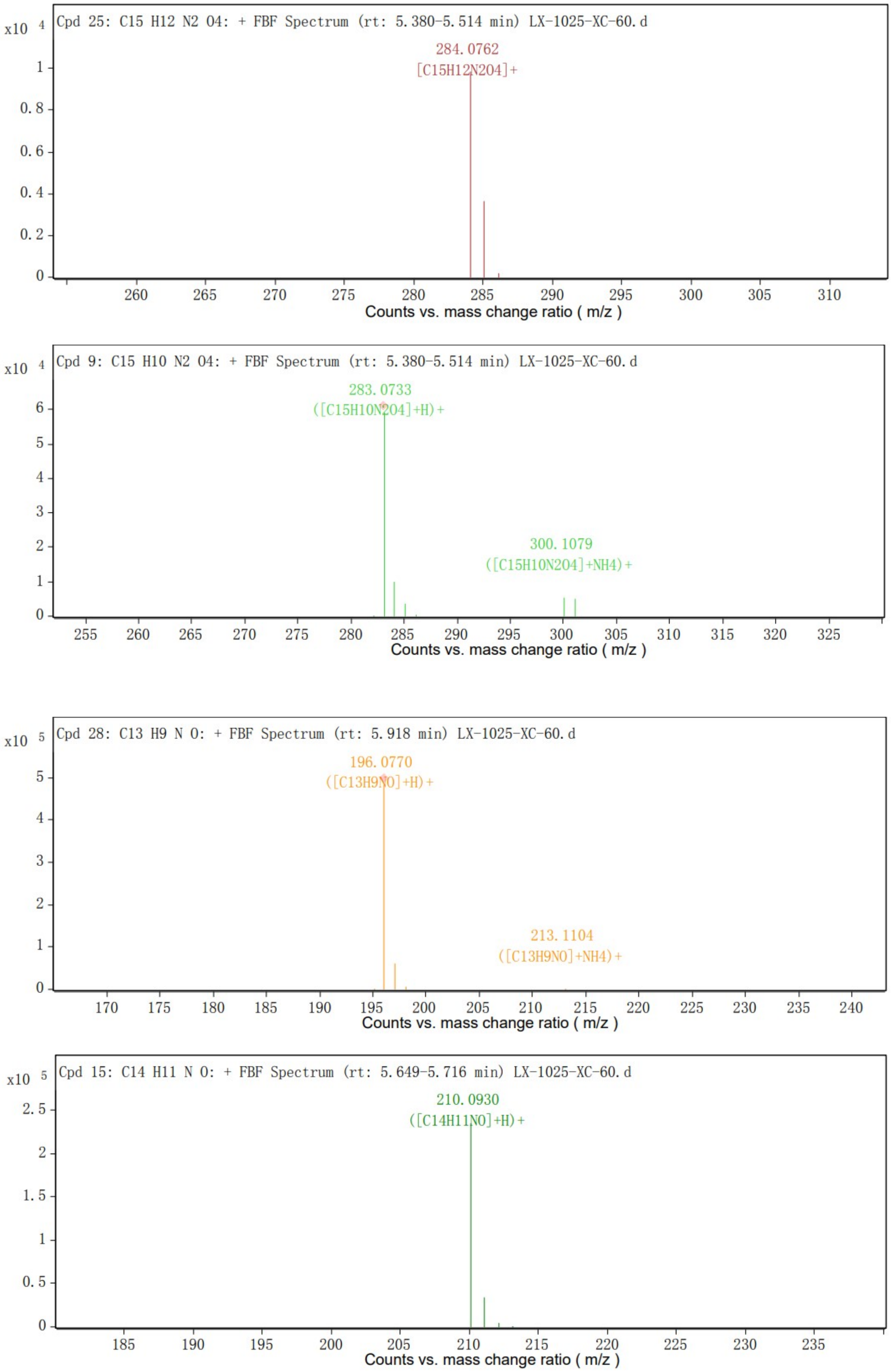
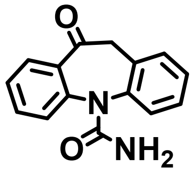
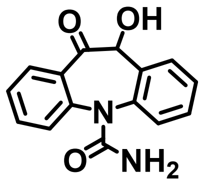
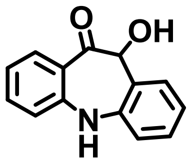
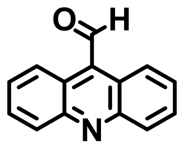
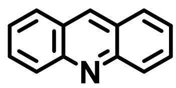
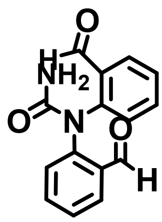
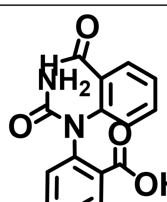
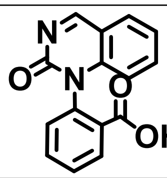
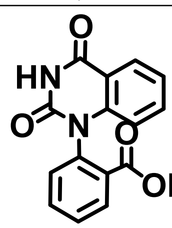
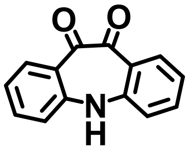
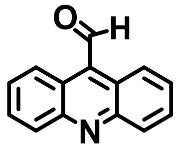
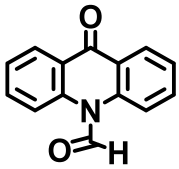
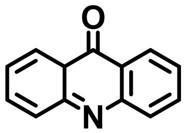
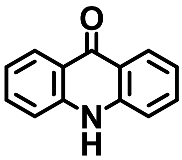
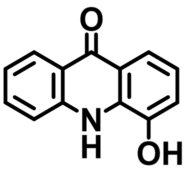


Fig. S14. HPLC-MS images of the degradation of OXC.

Table. S1. Possible degradation intermediates of OXC.

	m/z	Molecular structure	Molecular formular
OXC	252		$C_{15}H_{12}N_2O_2$
P1	268		$C_{15}H_{12}N_2O_3$
P2	225		$C_{14}H_{11}NO_2$
P3	207		$C_{14}H_9NO$
P4	179		$C_{13}H_9N$
P5	268		$C_{15}H_{12}N_2O_3$
P6	284		$C_{15}H_{12}N_2O_4$
P7	266		$C_{15}H_{10}N_2O_3$
P8	282		$C_{15}H_{10}N_2O_4$

P9	223		$C_{14}H_9NO_2$
P10	223		$C_{14}H_9NO_2$
P11	223		$C_{14}H_9NO_2$
P12	195		$C_{13}H_9NO$
P13	195		$C_{13}H_9NO$
P14	211		$C_{13}H_9NO_2$