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Supporting Information

Crystal facet and Na-doping dual engineering of bismuth oxychloride ultrathin nanosheets with efficient oxygen activation for enhanced photocatalytic performance

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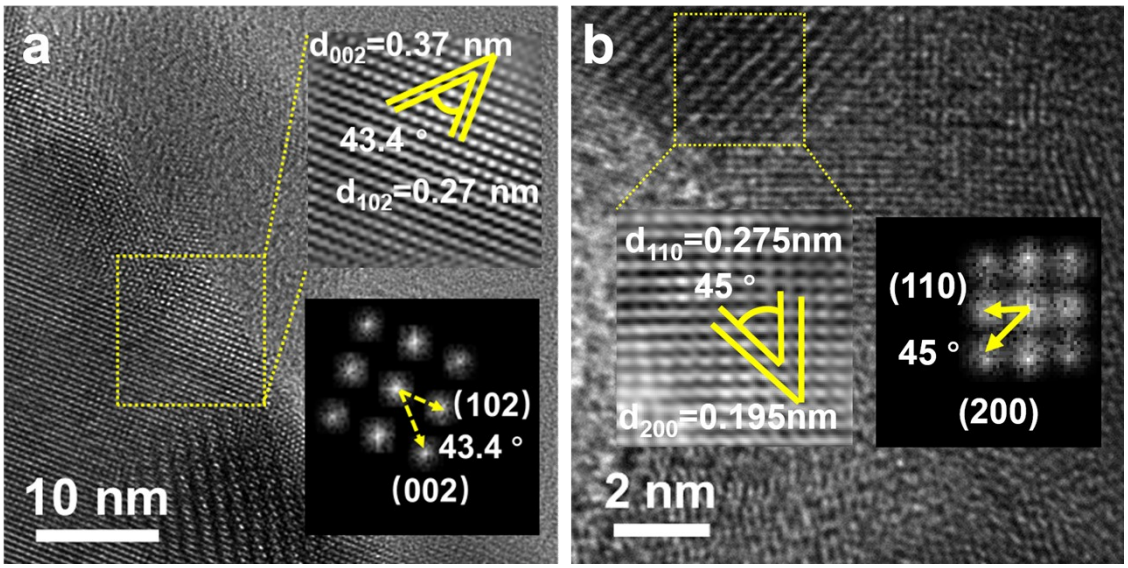


Fig. S1. HRTEM images with enlarged view (inset) and SAED patterns (inset) of (a) BOC-010 and (b) BOC-001.

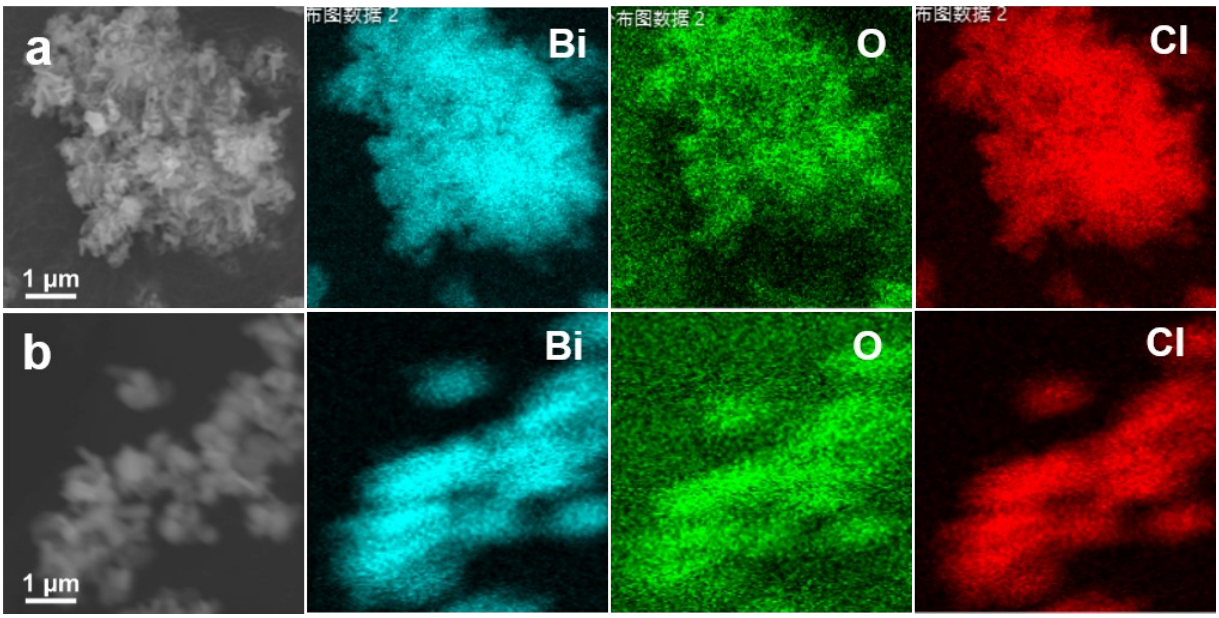


Fig. S2. SEM images and corresponding EDS elemental mapping of (a) BOC-010 and (b) BOC-001.

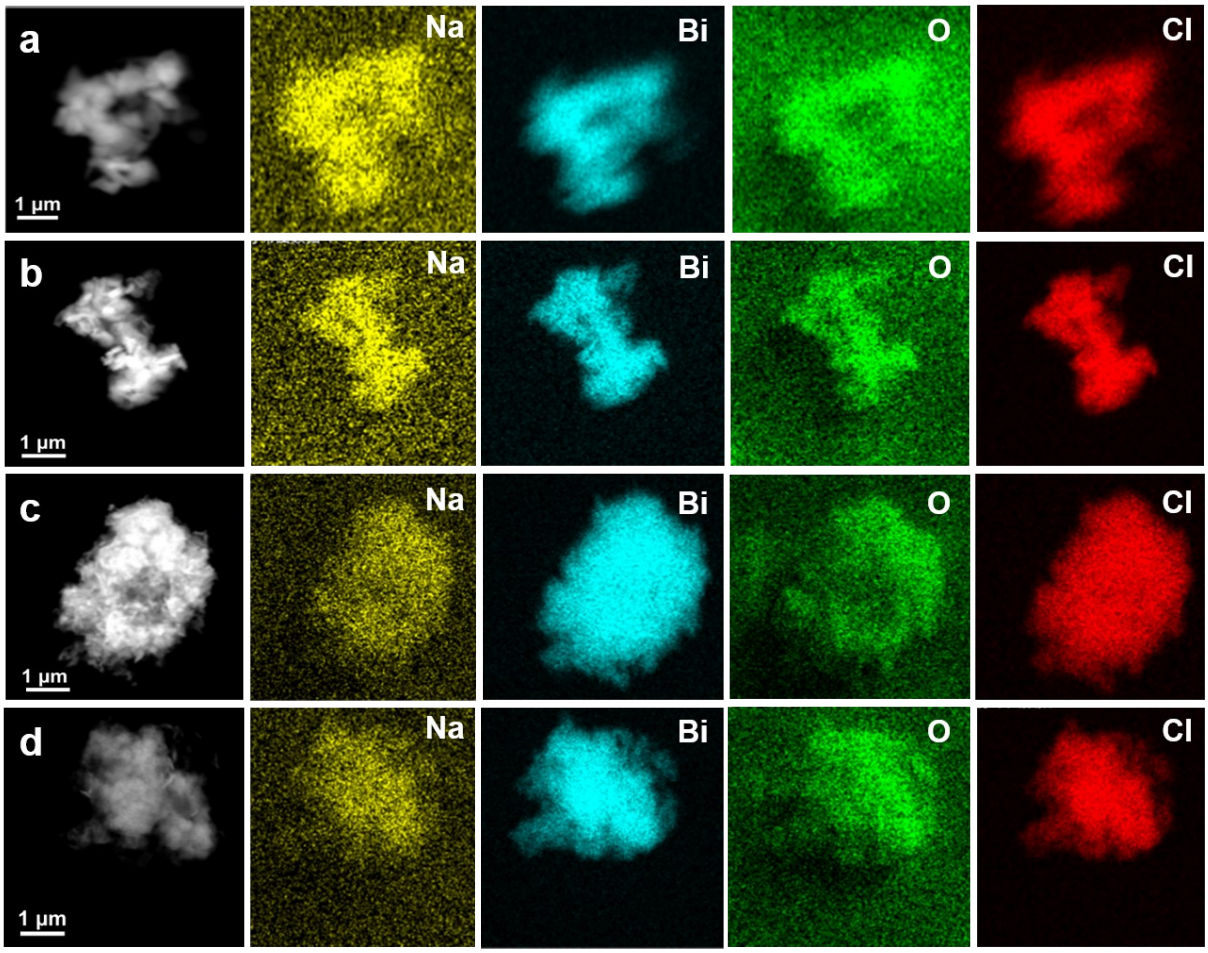


Fig. S3. SEM images and corresponding EDS elemental mapping of (a) 0.50-Na-BOC-010, (b) 0.15-Na-BOC-001, (c) 0.35-Na-BOC-001 and (d) 0.60-Na-BOC-001.

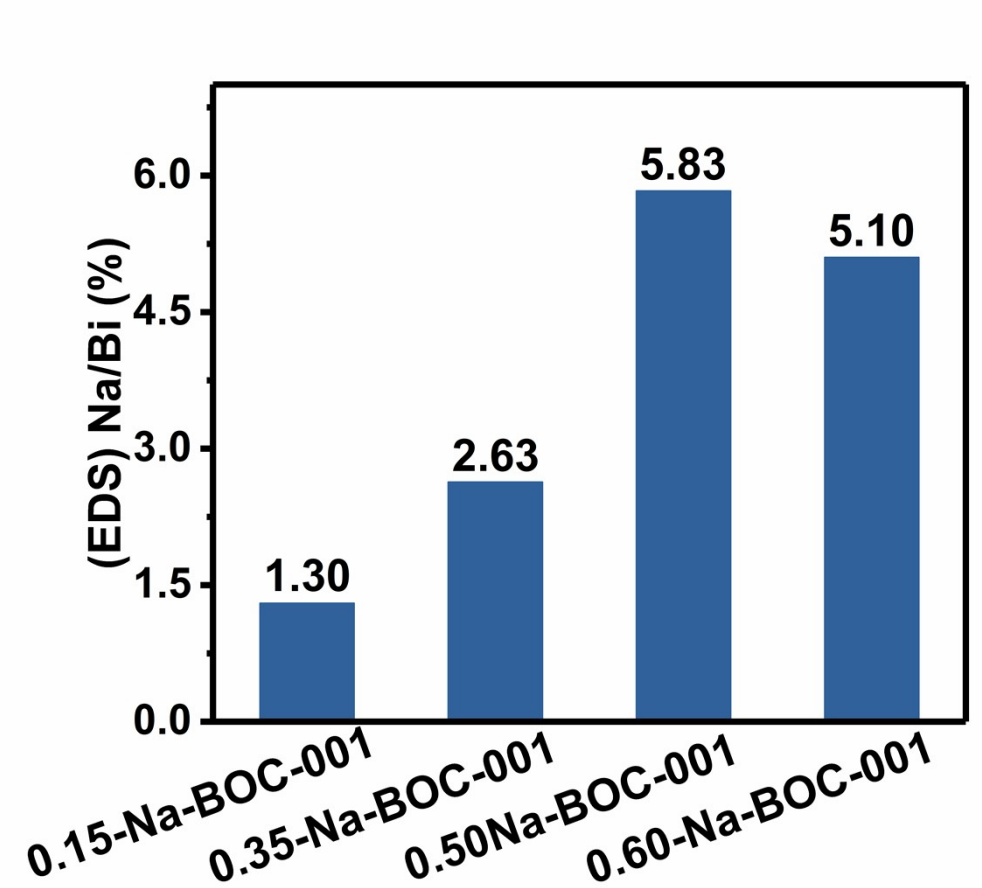


Fig. S4. (EDS) Na/Bi ratio of 0.15-Na-BOC-001, 0.35-Na-BOC-001, 0.50-Na-BOC-001 and 0.60-Na-BOC-001.

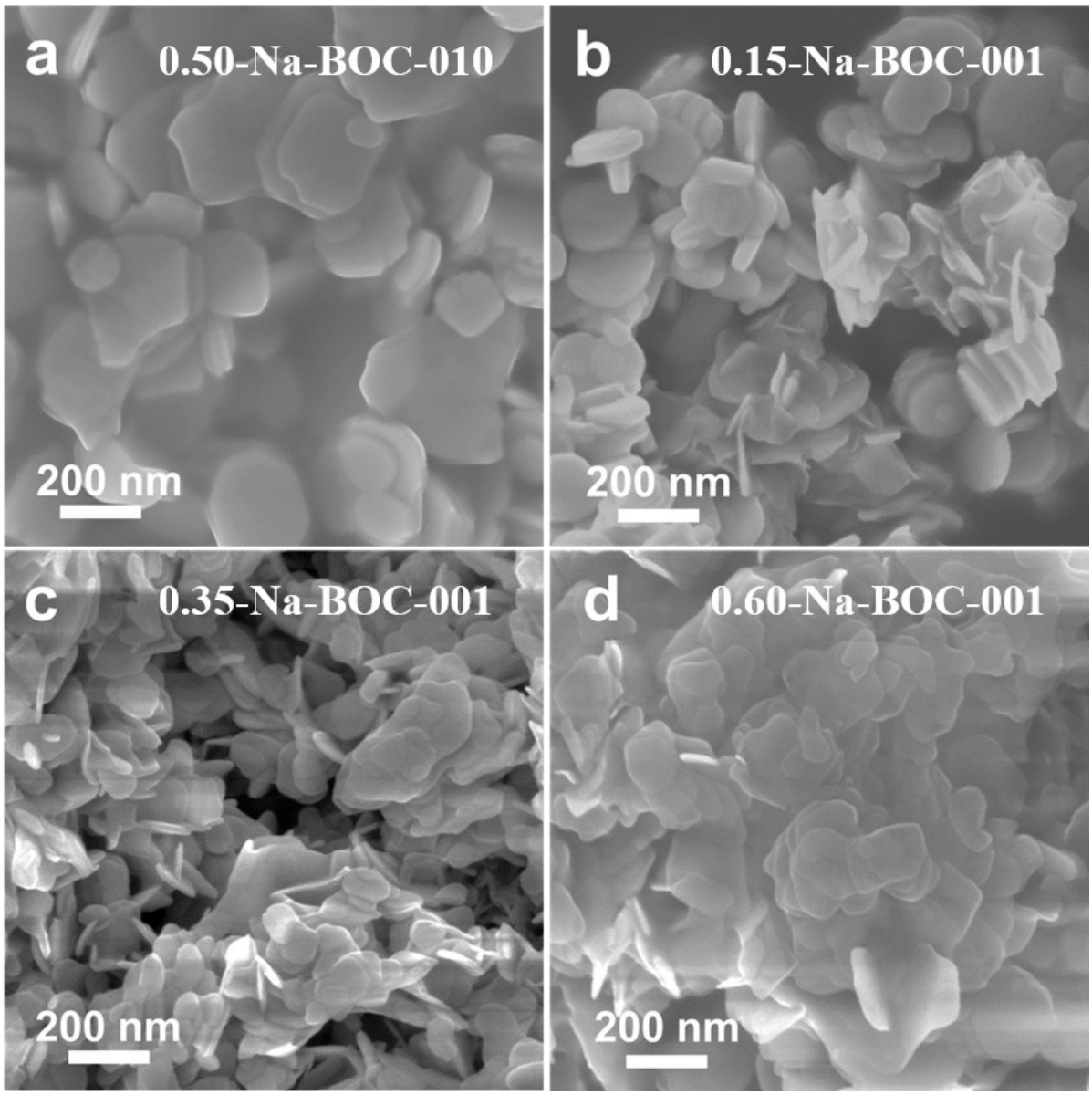


Fig. S5. SEM images of (a) 0.50-Na-BOC-010, (b) 0.15-Na-BOC-001, (c) 0.35-Na-BOC-001 and (d) 0.60-Na-BOC-001.

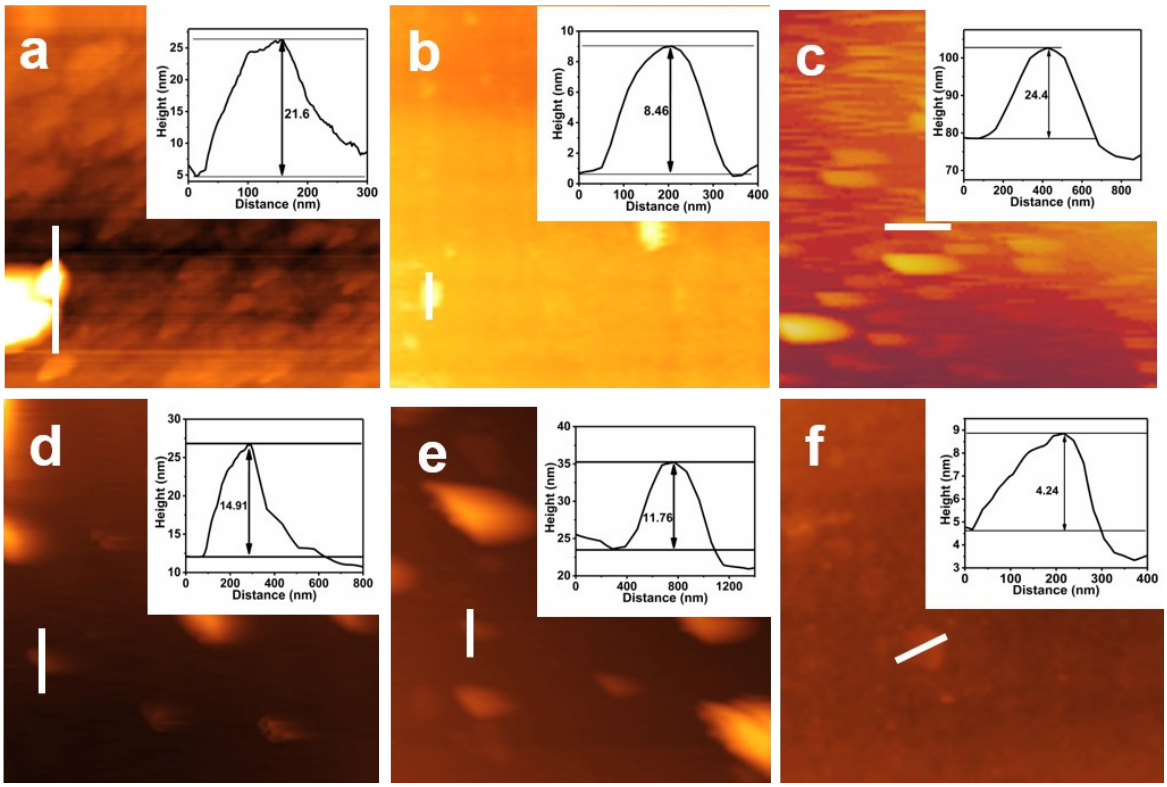


Fig. S6. AFM images and corresponding height profiles of (a) BOC-010, (b) BOC-001, (c) 0.50-Na-BOC-010, (d) 0.15-Na-BOC-001, (e) 0.35-Na-BOC-001 and 0.60-Na-BOC-001.

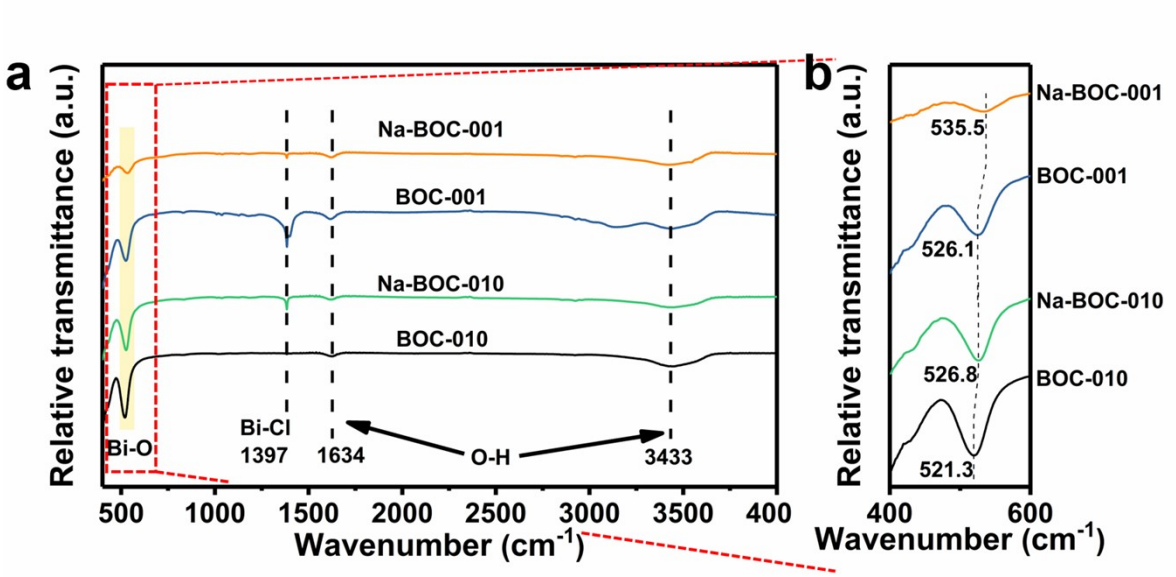


Fig. S7. FTIR spectra of BOC-010, Na-BOC-010, BOC-001 and Na-BOC-001 samples.

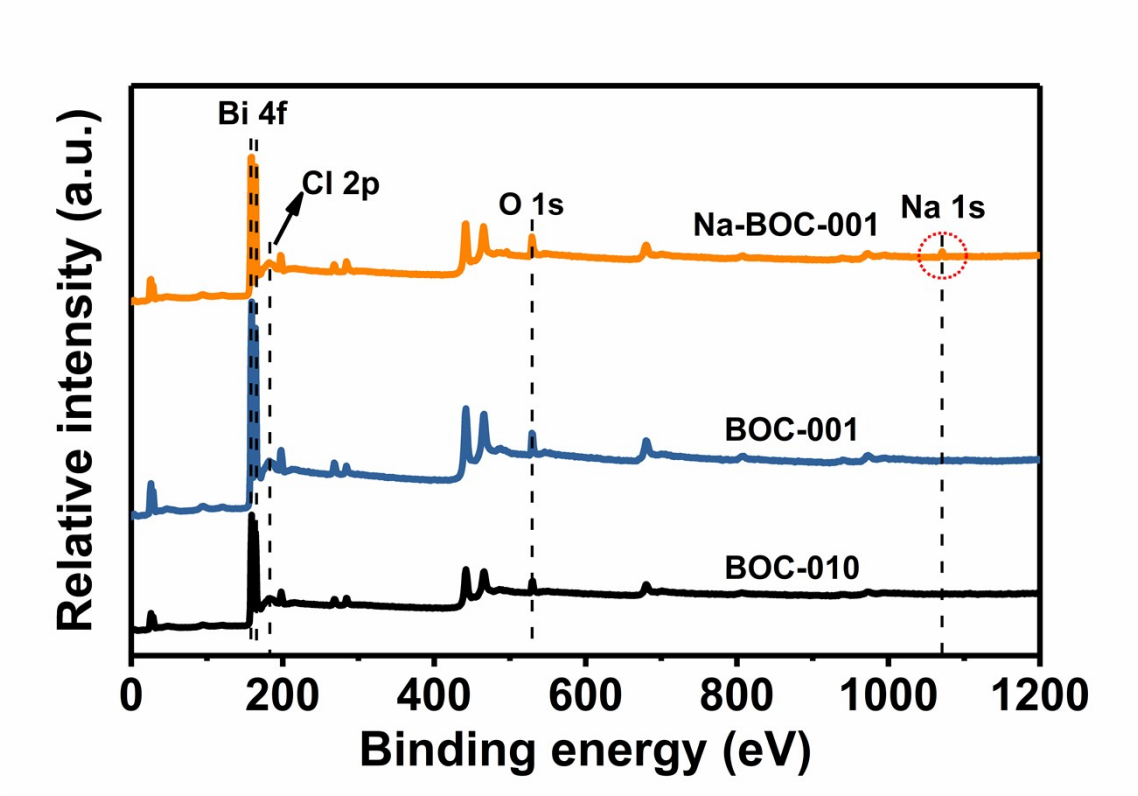


Fig. S8. Survey XPS spectra of BOC-010, BOC-001 and Na-BOC-001.

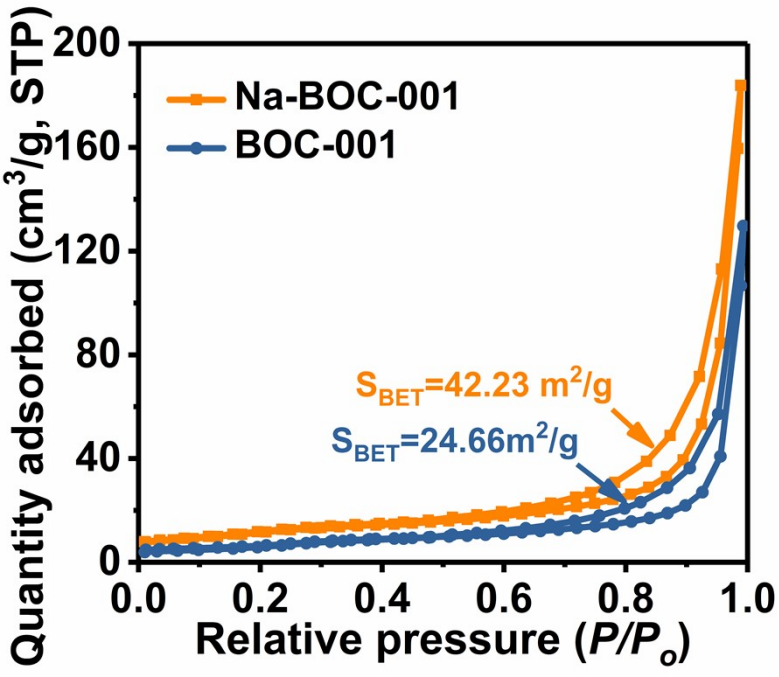


Fig. S9. N_2 adsorption and desorption isotherms of Na-BOC-001 and BOC-001.

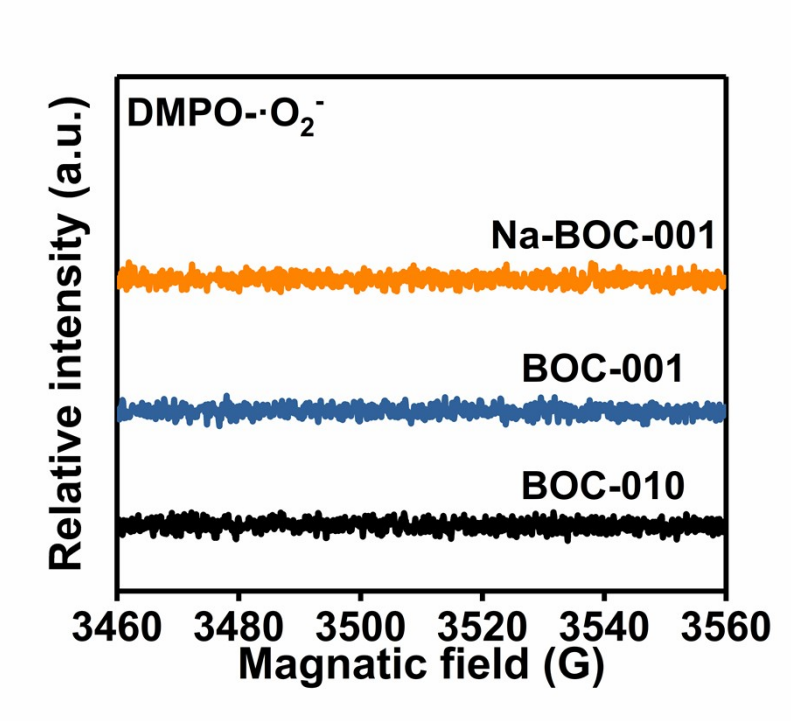


Fig. S10. ESR spectra of DMPO-•O_2^- over BOC-010, BOC-001, and Na-BOC-001 under darkness.

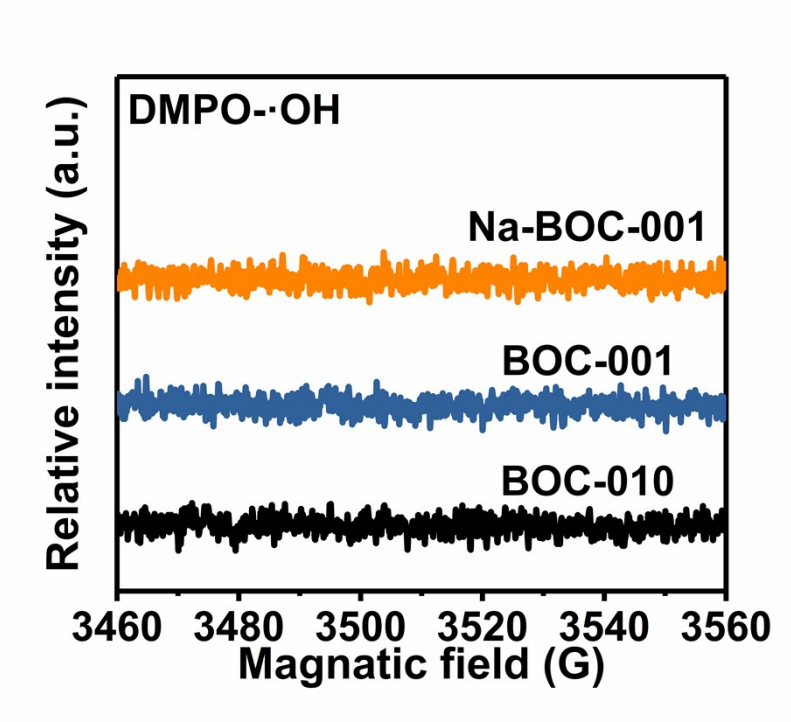


Fig. S11. ESR spectra of DMPO-•OH over BOC-010, BOC-001, and Na-BOC-001 under darkness.

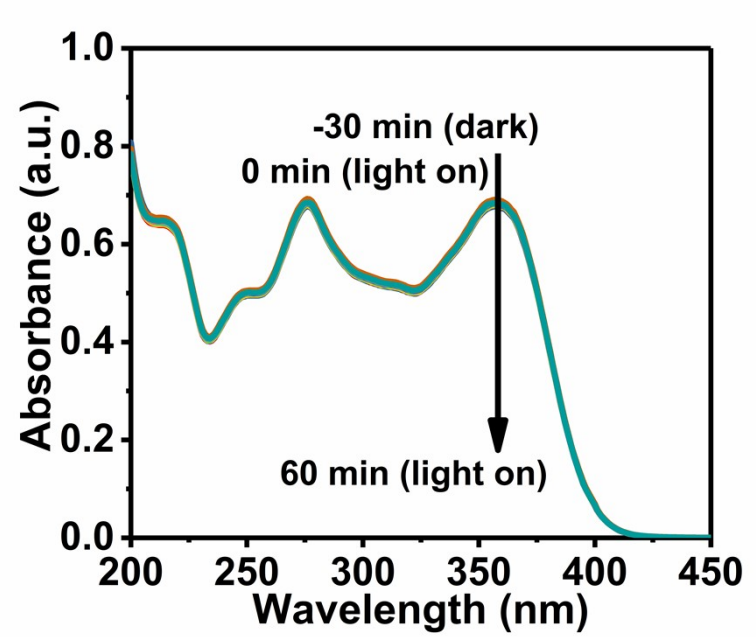


Fig. S12. UV-vis absorption spectra of TC collected during TC degradation process **without catalyst** with irradiation time (Conditions: [TC] = 20 mg L^{-1}, [catalyst] = 0 g L^{-1}, pH = 6.5, T = 25 °C, visible light (λ > 420 nm)).

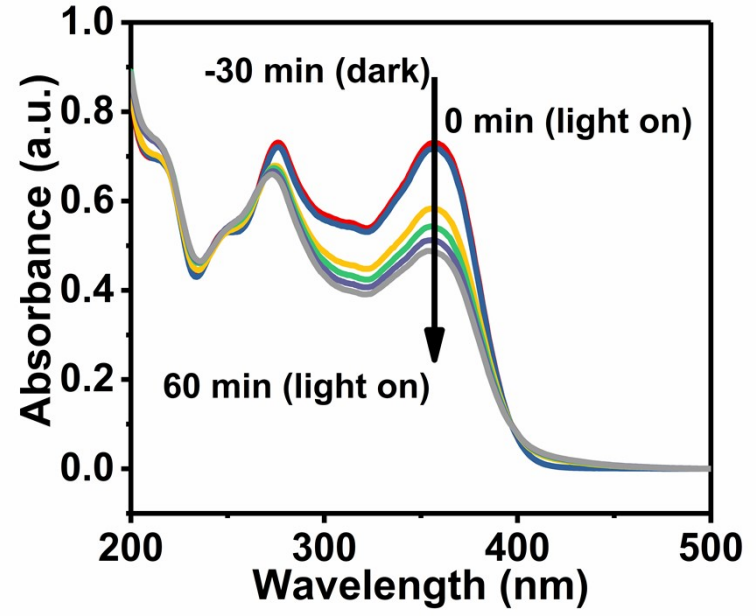


Fig. S13. UV-vis absorption spectra of TC collected during TC degradation process over **BOC-010** with irradiation time. (Conditions: [TC] = 20 mg L^{-1}, [catalyst] = 0.50 g L^{-1}, pH = 6.5, T = 25 °C, visible light (λ > 420 nm)).

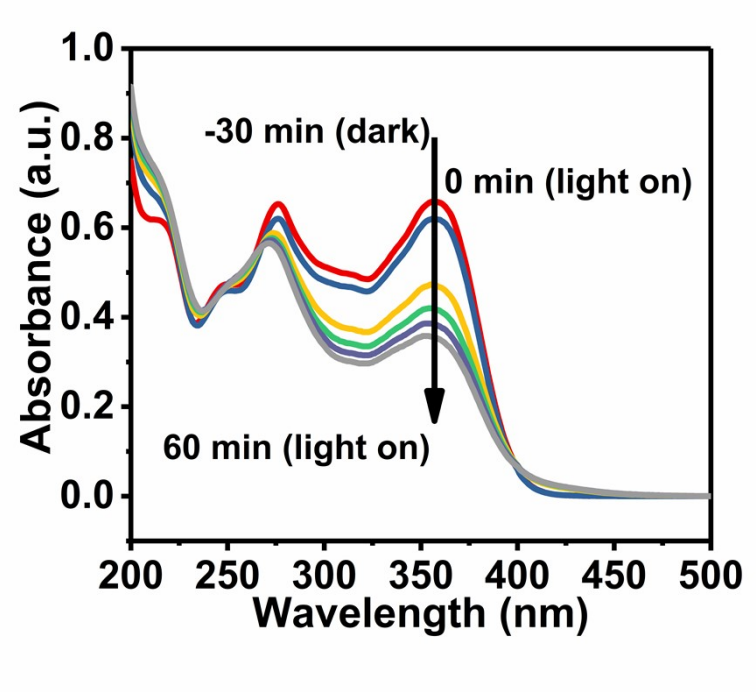


Fig. S14. UV-vis absorption spectra of TC collected during TC degradation process over **Na-BOC-010** with irradiation time. (Conditions: [TC] = 20 mg L^{-1}, [catalyst] = 0.50 g L^{-1}, pH = 6.5, T = 25 °C, visible light (λ > 420 nm)).

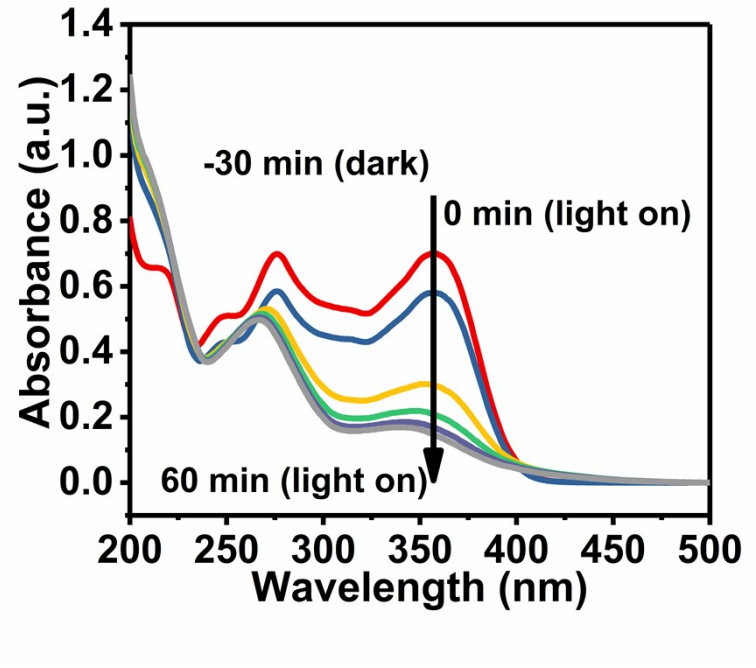


Fig. S15. UV-vis absorption spectra of TC collected during TC degradation process over **BOC-001** with irradiation time. (Conditions: [TC] = 20 mg L^{-1}, [catalyst] = 0.50 g L^{-1}, pH = 6.5, T = 25 °C, visible light (λ > 420 nm)).

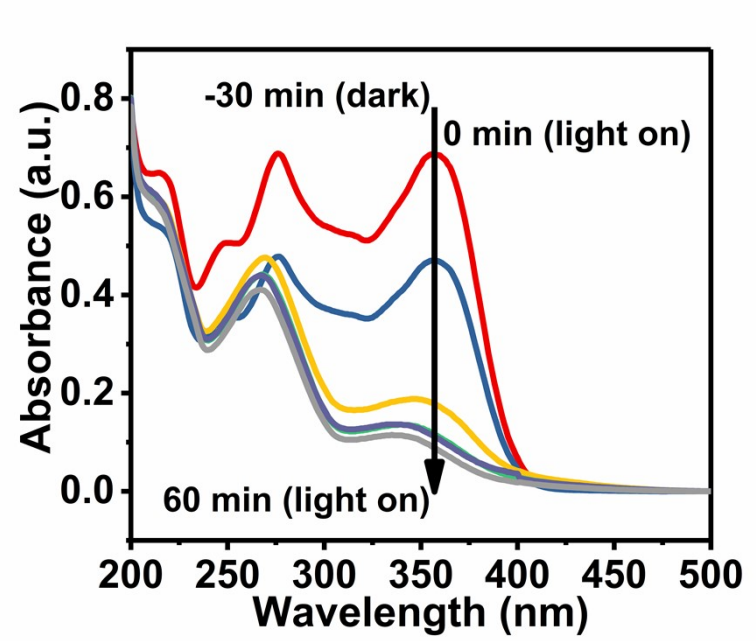


Fig. S16. UV-vis absorption spectra of TC collected during TC degradation process over **Na-BOC-001** with irradiation time. (Conditions: [TC] = 20 mg L^{-1}, [catalyst] = 0.50 g L^{-1}, pH = 6.5, T = 25 °C, visible light (λ > 420 nm)).

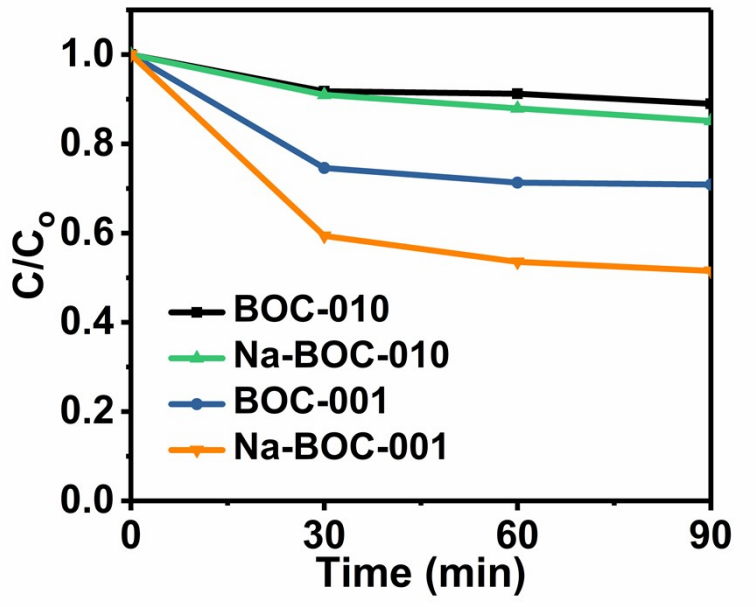


Fig. S17. TC adsorption profiles over the samples (BOC-010, Na-BOC-010, BOC-001 and Na-BOC-001) under dark condition. (Conditions: [TC] = 20 mg L^{-1}, [catalyst] = 0.50 g L^{-1}, pH = 6.5, T = 25 °C, visible light (λ > 420 nm)).

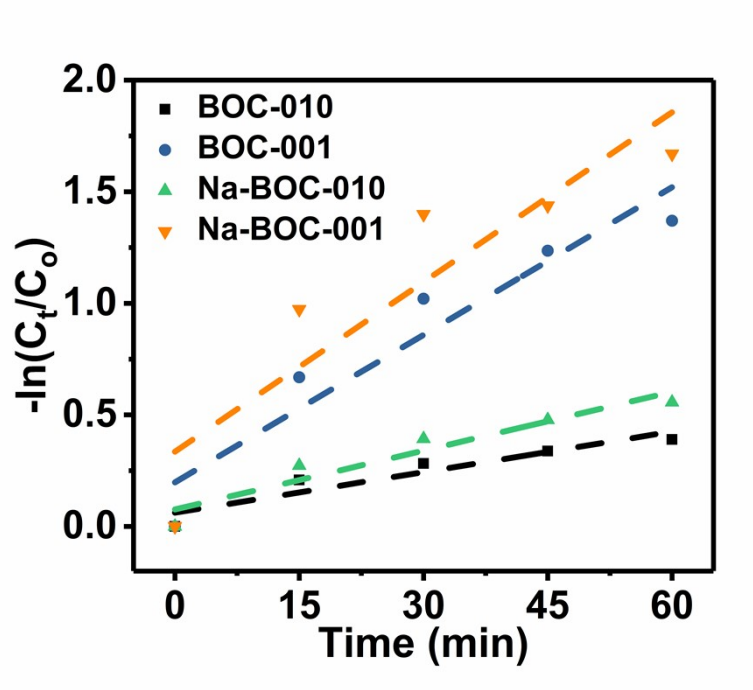
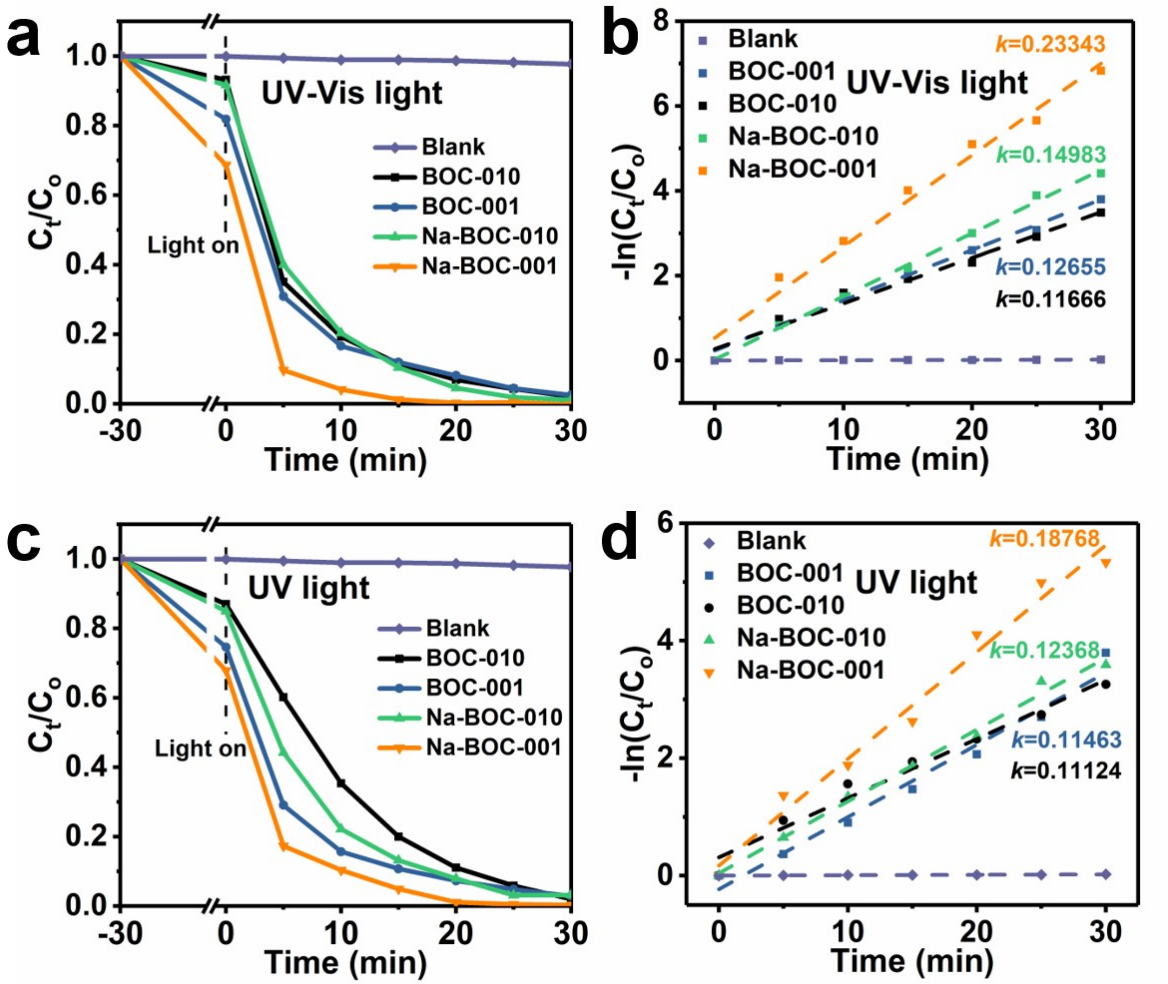


Fig. S18. Pseudo-first-order kinetic fitting curves and corresponding kinetic constants (*k*) over different samples under the irradiation of Vis light.



92

93 **Fig. S19.** (a) Photocatalytic degradation curves of TC and (b) Pseudo-first-order kinetic fitting curves and
94 corresponding kinetic constants (*k*) over different samples under the irradiation of UV-Vis light. (c)
95 Photocatalytic degradation curves of TC and (d) Pseudo-first-order kinetic fitting curves and corresponding
96 kinetic constants (*k*) over different samples under the irradiation of UV light. Conditions: [TC] = 20 mg L^{-1},
97 [catalyst] = 0.5 g L^{-1}, pH = 6.5, T = 25 °C, UV-Vis light (λ>320 nm), UV light (320<λ<420 nm).
98

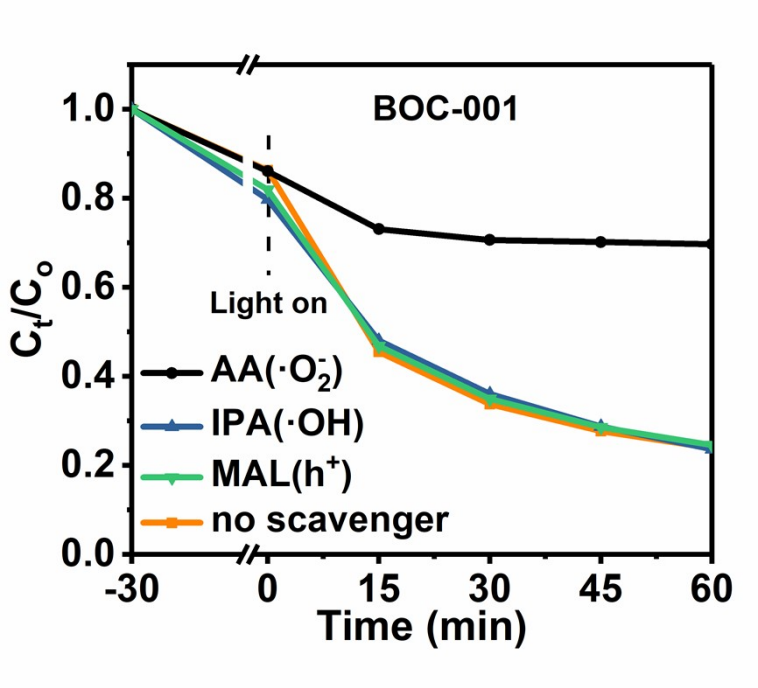


Fig. S20. TC removal profiles over **BOC-001** with addition of various radical sacrificial agents. Conditions: [TC] = 20 mg L^{-1}, [catalyst] = 0.5 g L^{-1}, pH = 6.5, T = 25 °C, visible light ($\lambda > 420$ nm).

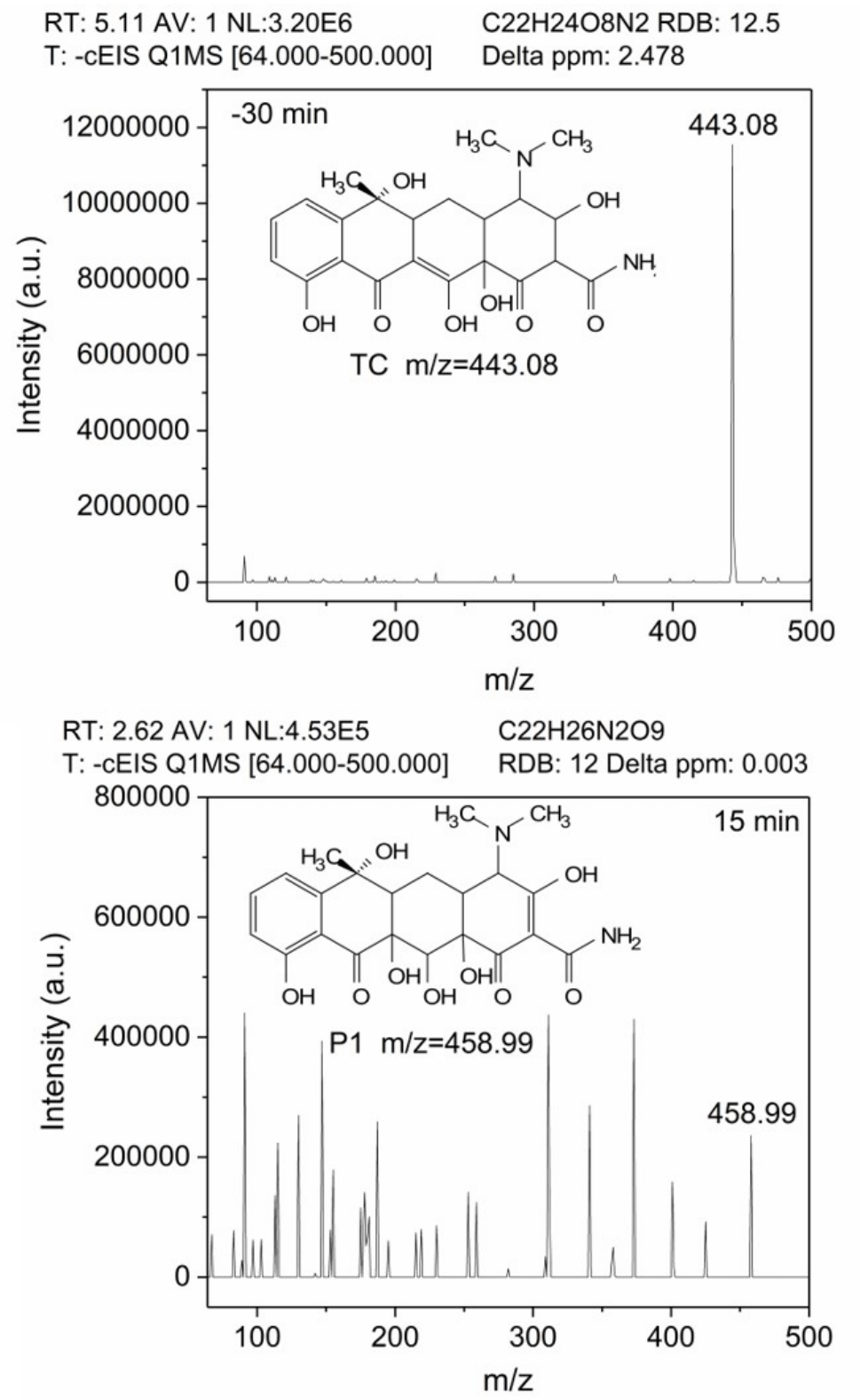


Fig. S21. MS spectra of identified **TC and P1** from solution collected during TC degradation process over Na-BOC-001 with different irradiation time.

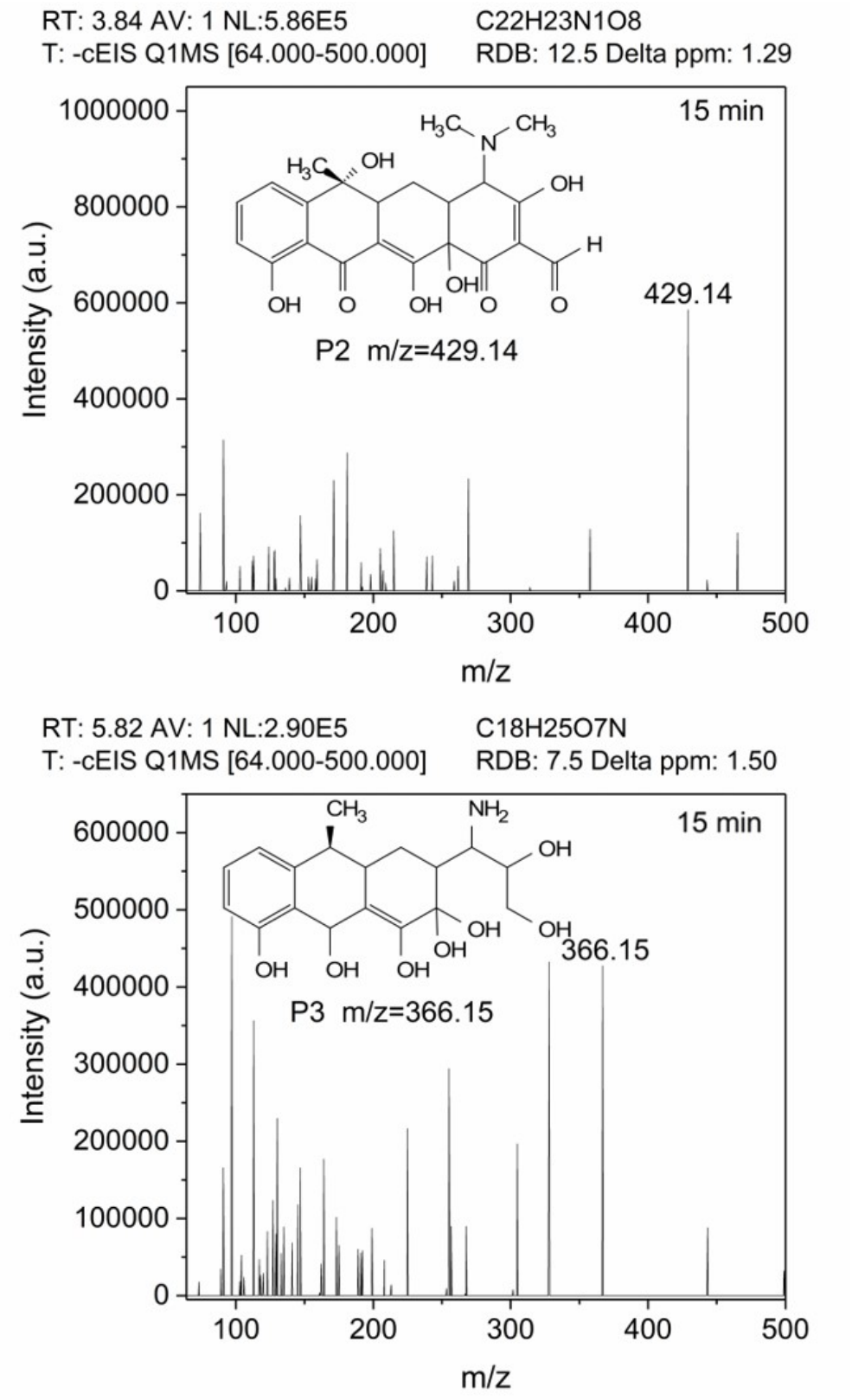


Fig. S22. MS spectra of identified **P2 and P3** from solution collected during TC degradation process over Na-BOC-001 at irradiation time of 15 min.

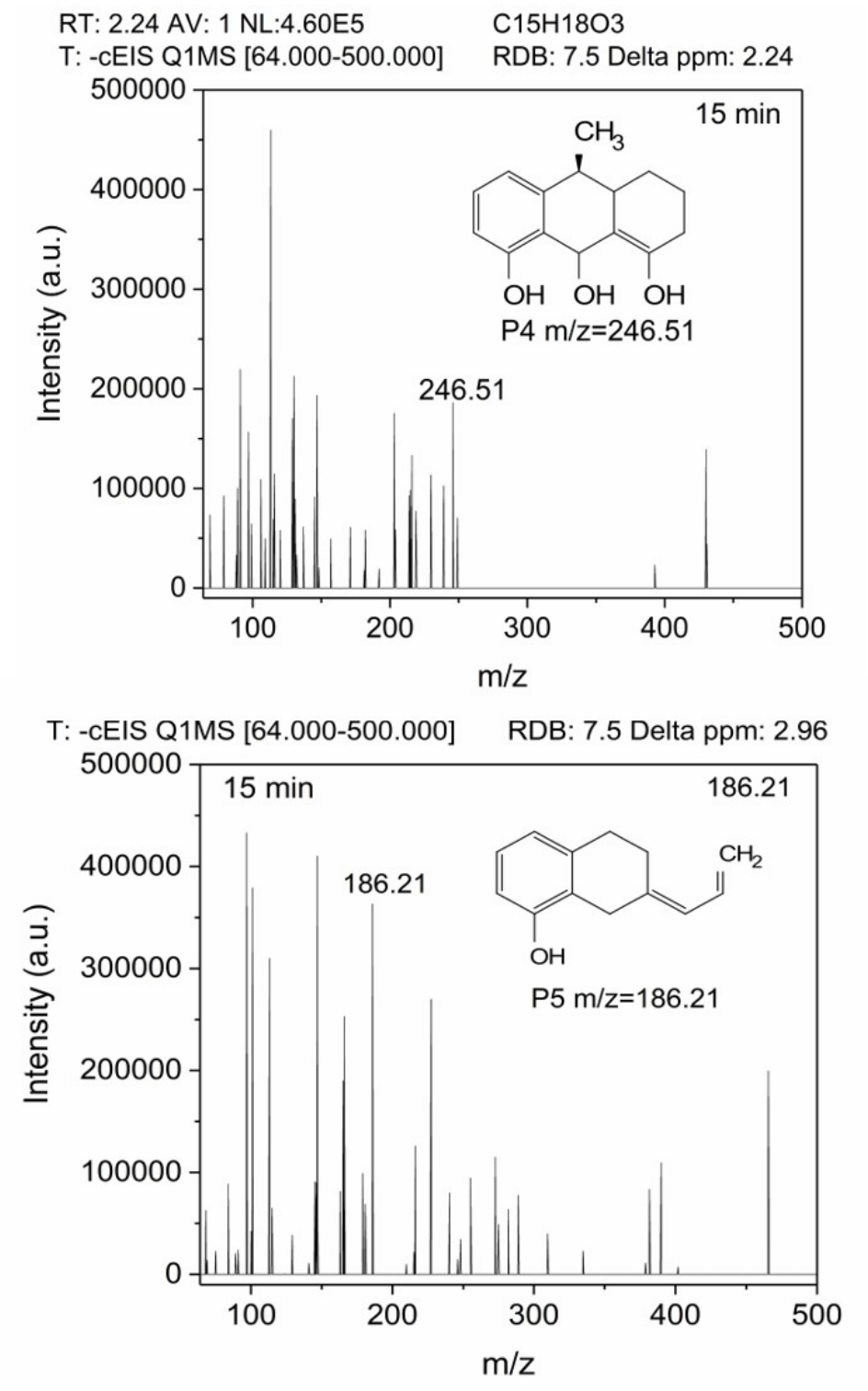


Fig. S23. MS spectra of identified **P4 and P5** from solution collected during TC degradation process over Na-BOC-001 at irradiation time of 15 min.

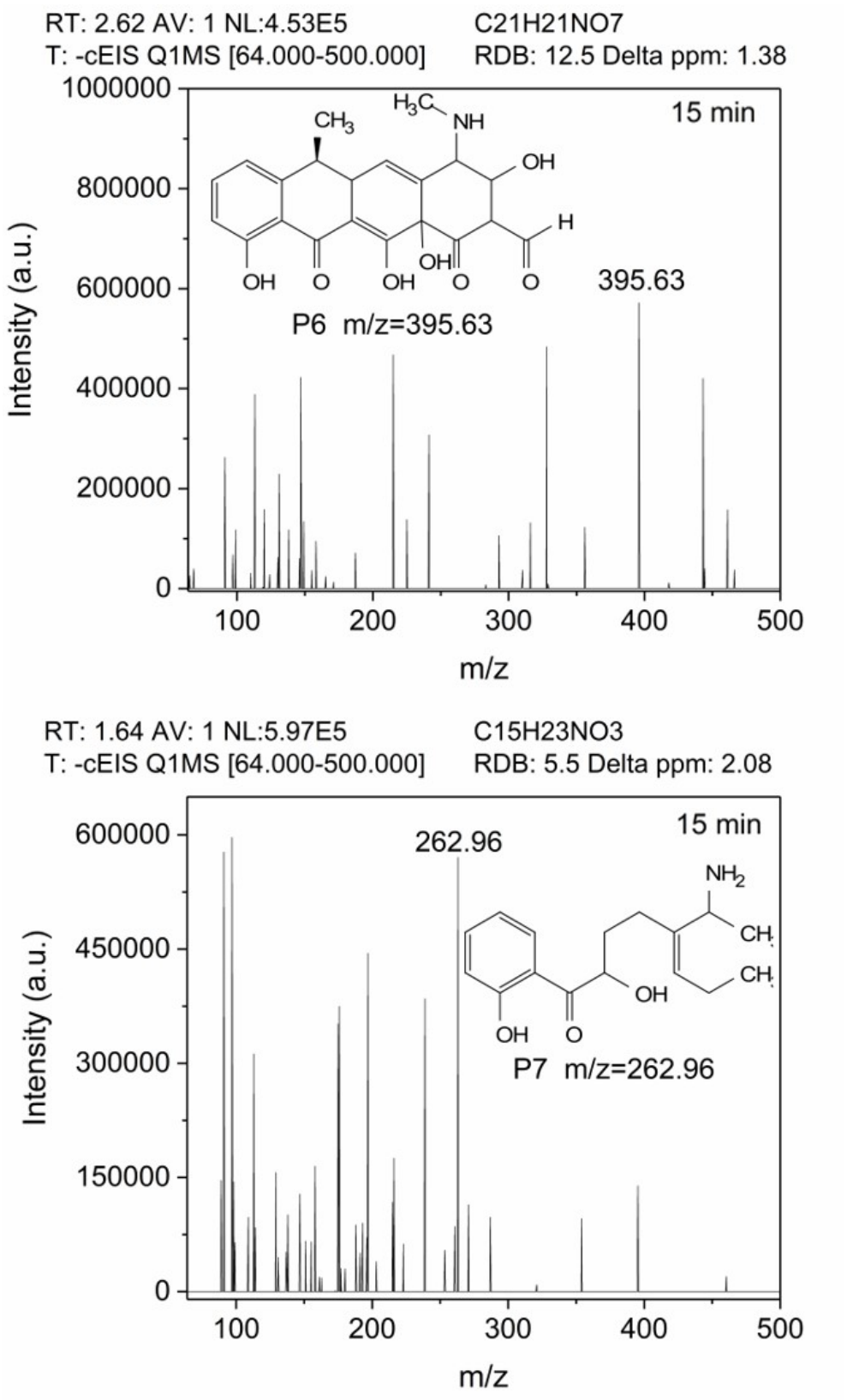


Fig. S24. MS spectra of identified **P6 and P7** from solution collected during TC degradation process over Na-BOC-001 at irradiation time of 15 min.

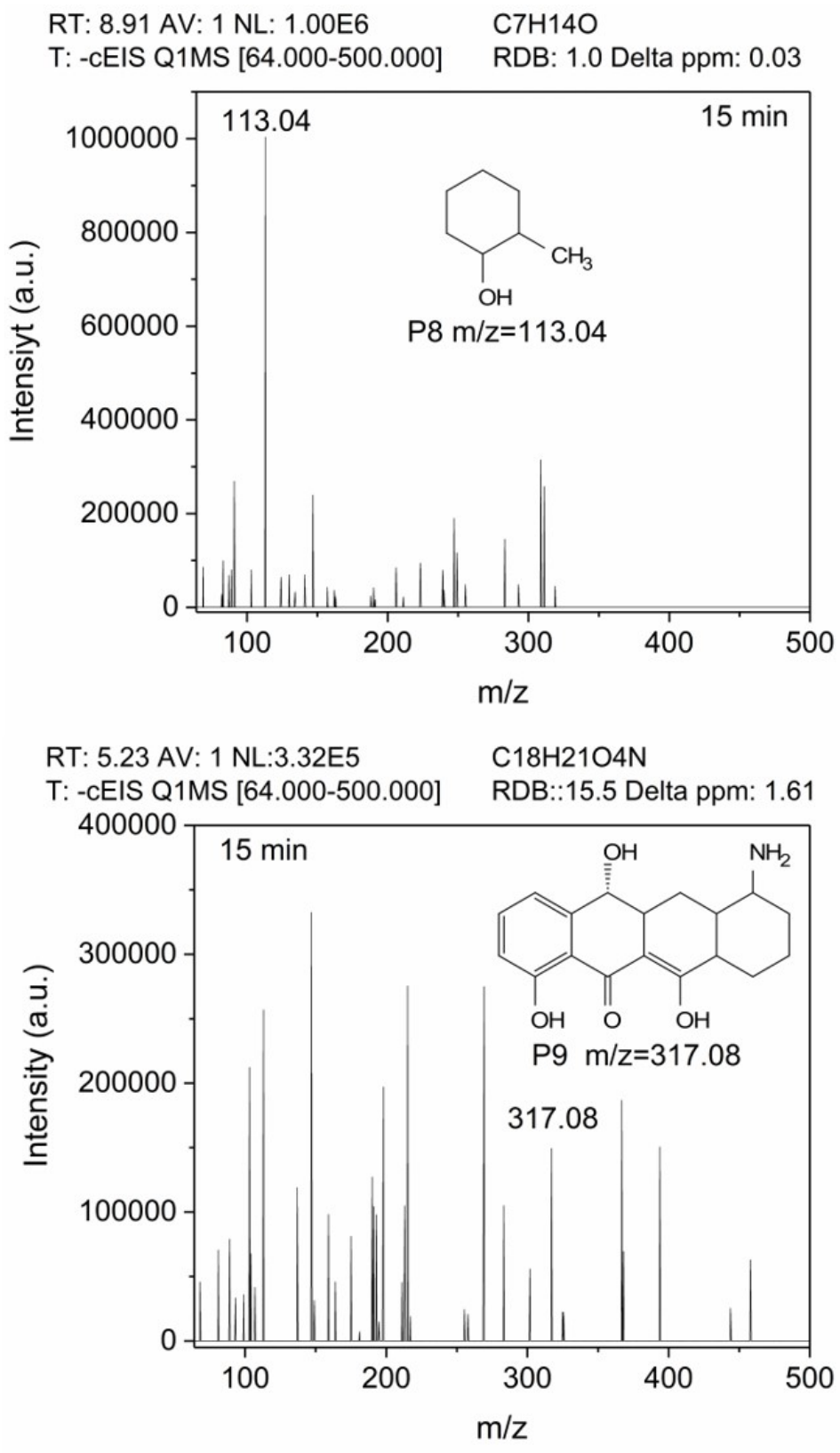


Fig. S25. MS spectra of identified **P8 and P9** from solution collected during TC degradation process over Na-BOC-001 at irradiation time of 15 min.

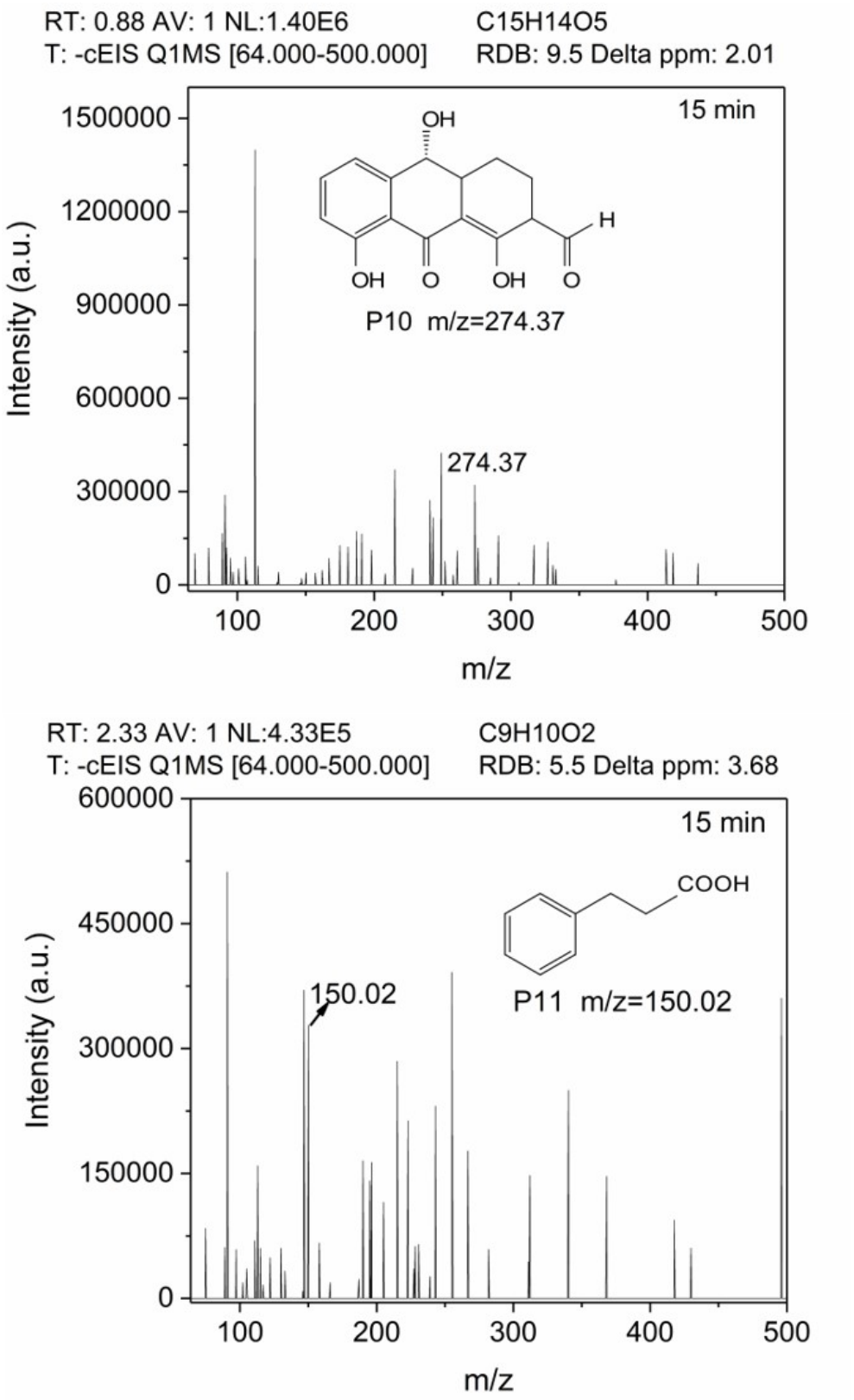


Fig. S26. MS spectra of identified **P10 and P11** from solution collected during TC degradation process over Na-BOC-001 at irradiation time of 15 min.

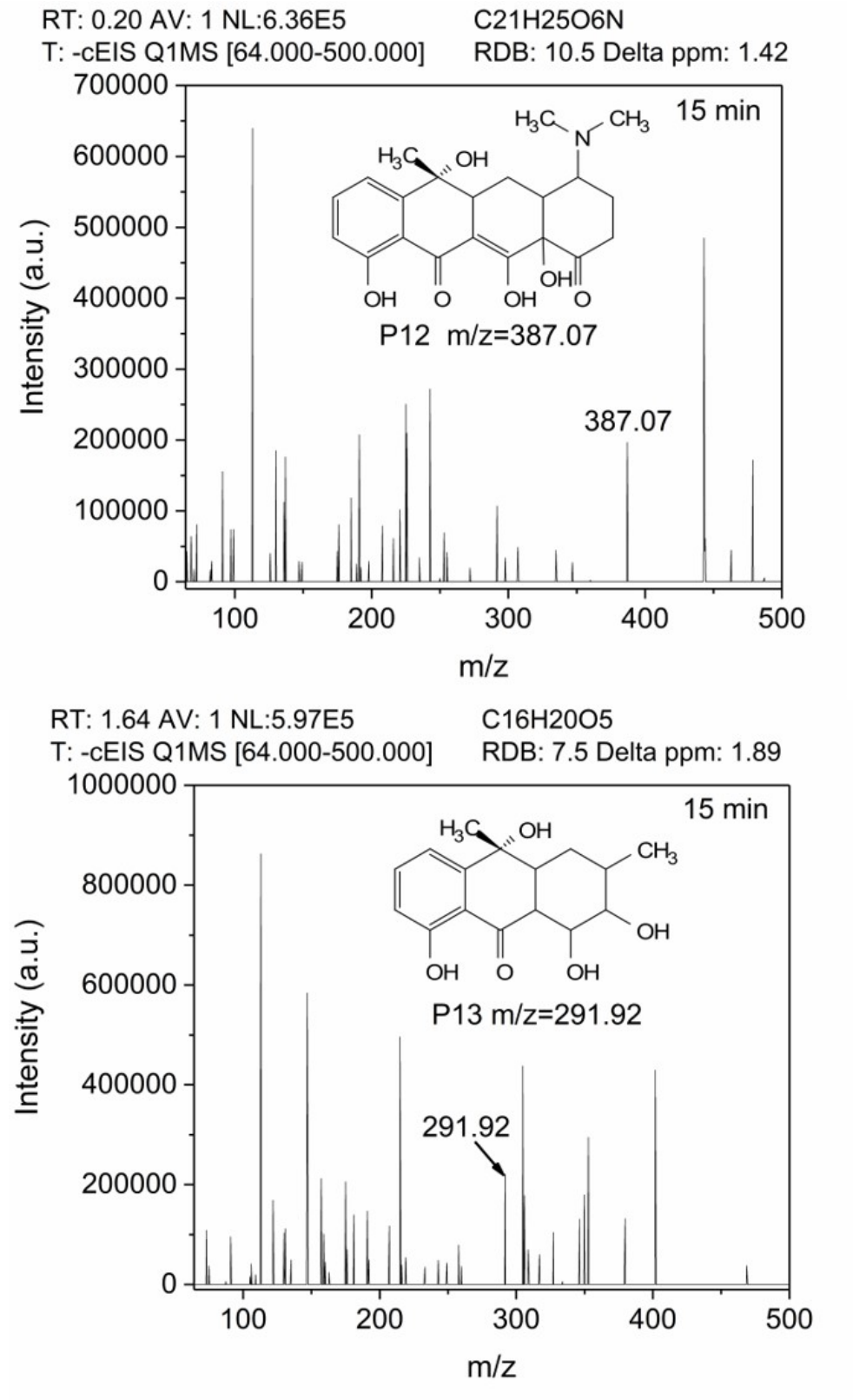
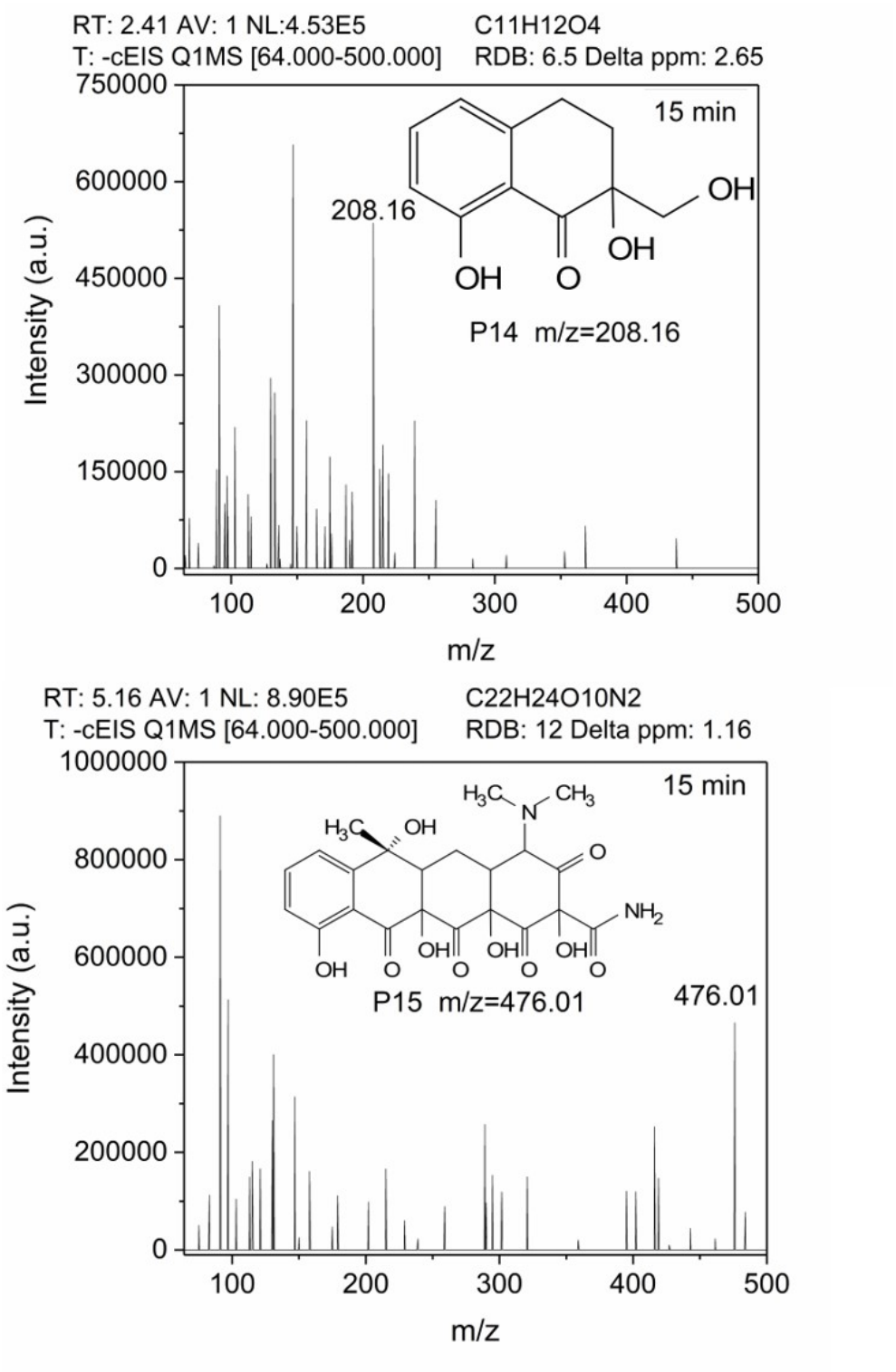


Fig. S27. MS spectra of identified **P12 and P13** from solution collected during TC degradation process over Na-BOC-001 at irradiation time of 15 min.



125

126 **Fig. S28.** MS spectra of identified **P14 and P15** from solution collected during TC
127 degradation process over Na-BOC-001 at irradiation time of 15 min.

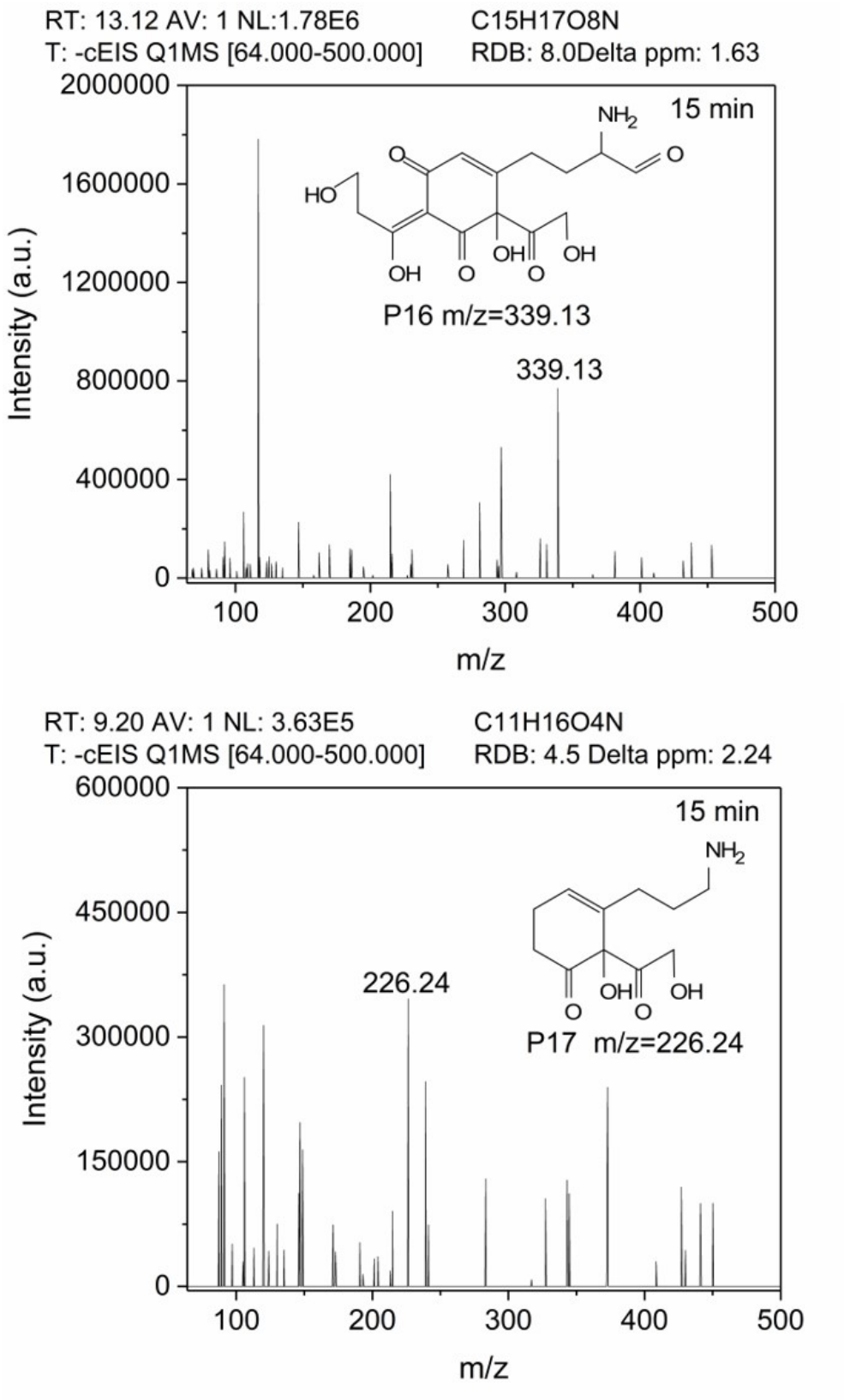
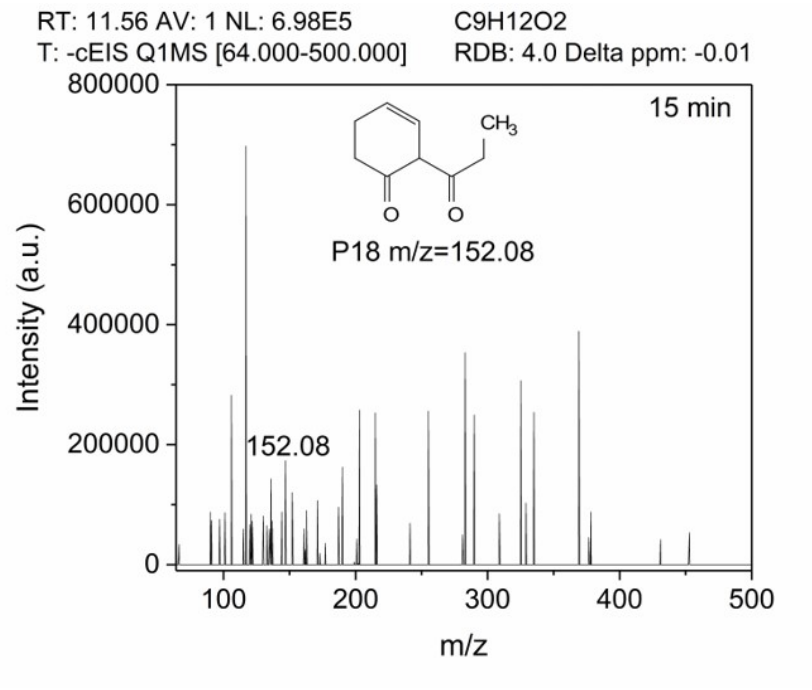
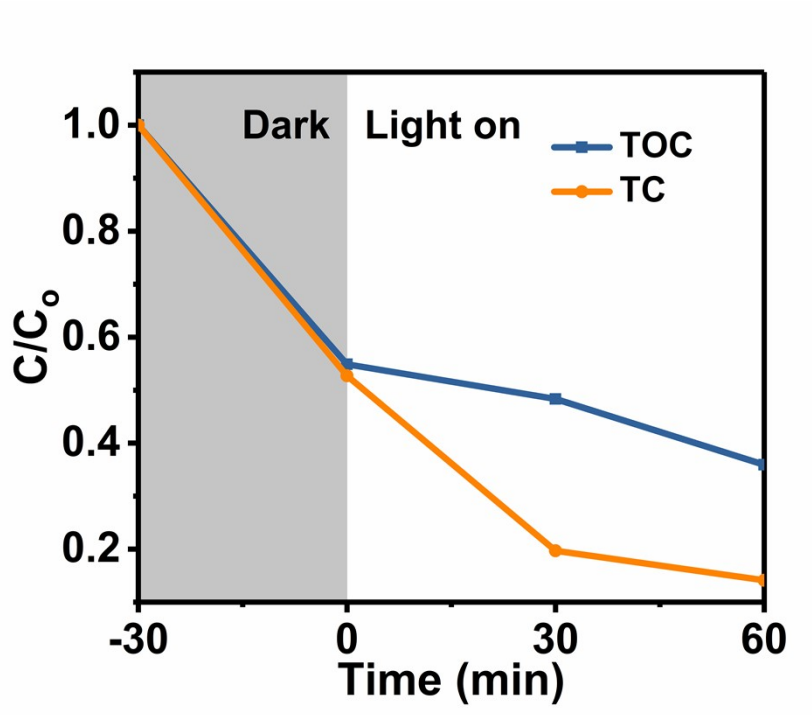


Fig. S29. MS spectra of identified **P16 and P17** from solution collected during TC degradation process over Na-BOC-001 at irradiation time of 15 min.



131

132 **Fig. S30.** MS spectra of identified **P18** from solution collected during TC degradation process
133 over Na-BOC-001 at irradiation time of 15 min.



134

135 **Fig. S31.** TOC concentration and TC removal profiles in the TC solution versus time during
136 the photocatalysis process over Na-BOC-001. Conditions: [TC] = 20 mg L^{-1}, [catalyst] =0.5 g
137 L^{-1}, pH = 6.5, T=25 °C, visible light (λ>420 nm).

Table S1 Elemental composition of as-prepared samples detected by EDS.

Sample	Relative Content (at. %)				Na/Bi (%)
	Na	Bi	O	Cl	
BOC-010		11.71	76.47	11.81	
BOC-001		22.16	58.91	18.93	
0.50-Na-BOC-010	0.20	6.77	86.44	6.59	**2.95**
0.15-Na-BOC-001	0.11	8.45	83.26	8.18	**1.30**
0.35-Na-BOC-001	0.32	12.16	76.73	10.79	**2.63**
0.50-Na-BOC-001	1.56	26.77	48.79	21.87	**5.83**
0.60-Na-BOC-001	0.53	10.39	79.22	9.86	**5.10**

Table S2 Relative percent content of lattice oxygen, oxygen vacancy and surface adsorbed oxygen peaks in the as-prepared samples by O 1s XPS spectral fitting.

Sample	Lattice oxygen (O_α)			Oxygen vacancy (O_β)			Surface adsorbed oxygen (O_ε)		
	Peak (eV)	Area	*O_α/O_T (%)	Peak (eV)	Area	*O_β/O_T (%)	Peak (eV)	Area	*O_ε/O_T (%)
BOC-010	529.9	44140	71.0	531.3	11295	18.2	533.1	6721	10.8
BOC-001	529.9	86677	75.3	531.3	19399	16.9	533.1	8914	7.8
Na-BOC-001	529.7	70814	70.9	531.1	6986	7.0	532.7	22042	22.1

* $O_T = O_\alpha + O_\beta + O_\varepsilon$

Table S3 Kinetic fitting data of TC degradation over as-prepared samples under the irradiation of UV-Vis light.

Samples	Kinetic Equation	Kinetics Rate (k, min^{-1}) *	R^2
BOC-010	y=0.27303+0.10756x	0.11666	0.97839
BOC-001	y=0.23589+0.11869x	0.12655	0.98763
Na-BOC-010	y=0.02439+0.14902x	0.14983	0.99751
Na-BOC-001	y=0.53512+0.21560x	0.23343	0.98061

*$\ln(C_o/C_t)=k_{app}t$ [1]

Table S4 Kinetic fitting data of TC degradation over as-prepared samples under the irradiation of UV light.

Samples	Kinetic Equation	Kinetics Rate (k, min^{-1}) *	R^2
BOC-010	y=0.31041+0.10089x	0.11124	0.96718
BOC-001	y=0.31041+0.10089x	0.11463	0.97752
Na-BOC-010	y=0.04282+0.12225x	0.12368	0.99253
Na-BOC-001	y=0.17090+0.18198x	0.18768	0.98114

*$\ln(C_o/C_t)=k_{app}t$ [1]

Table S5 Kinetic fitting data of TC degradation over as-prepared samples under the irradiation of Vis light.

Samples	Kinetic Equation	Kinetics Rate (k, min^{-1}) *	R^2
BOC-010	y=0.06176+0.00605x	0.00708	0.89510
BOC-001	y=0.19743+0.02205x	0.02534	0.90903
Na-BOC-010	y=0.07620+0.00878x	0.01005	0.92054
Na-BOC-001	y=0.33510+0.02536x	0.03095	0.82498

*$\ln(C_o/C_t)=k_{app}t$ [1]

Table S6 Kinetic fitting data of TC degradation over as-prepared samples.

Photocatalysts	Contaminant	Light sources	Dosage (g L^{-1})	C_0 (mg L^{-1})	Volume (mL)	Time (min)	Degradation rates (%)	Ref.
Na-BOC-001	TC	Vis	0.5	20	100	60	87.2	This work
$WO_3/Bi_{12}O_{17}Cl_2$	TC	Vis	0.8	20	80	180	63.2	1
BiOCl/CAU-17	TC	Xenon	0.1	10	100	90	85.5	2
NH_2-MIL-125 (Ti)/BiOCl	TC	Vis	0.5	20	100	120	78.0	3
P-BiOCl	TC	Xenon	0.5	20	100	30	81.0	4

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