Electronic supplementary materials

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N-doping offering higher photodegradation performance of dissolved black carbon for organic pollutants: experimental and theoretical studies

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This supporting information contains three tables and 15 figures.

S1 Quantum yield calculation

The QY of GQDs was determined by using quinine sulfate as the standard sample and was calculated according to Eq. (S1).

$$Q = Q_r \times \frac{I}{I_r} \times \frac{A_r}{A} \times \left(\frac{n}{n_r} \right)^2 \quad \text{(S1)}$$

where Q is the quantum yield, I is the measured integrated emission intensity, n is the refractive index of the solvent (1.33 for water), and A is the optical density. The subscript "r" refers to the reference standard with known QY (Cai et al., 2014).

Reference

Cai F, Liu XD, Liu S, et al., 2014. A simple one-pot synthesis of highly fluorescent nitrogen-doped graphene quantum dots for the detection of Cr(VI) in aqueous media. *RSC Advances*, 4:52016-52022.

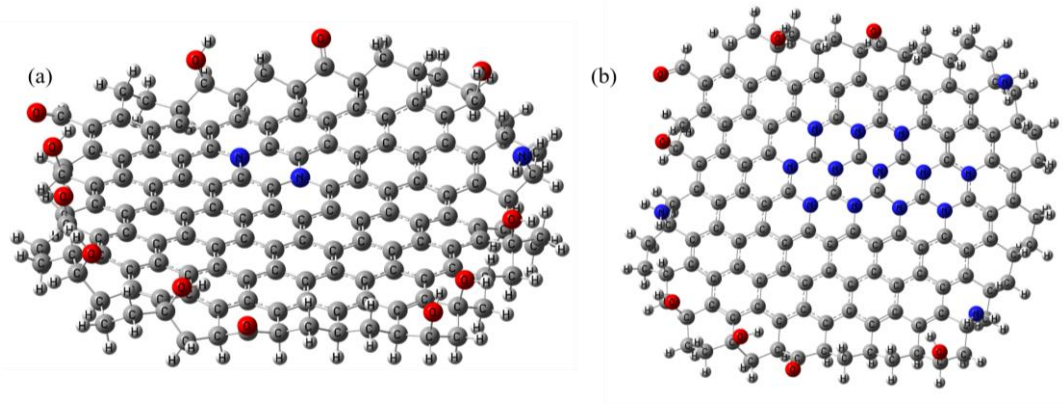


Fig. S1 the optimized molecular structure of (a) DBC model; (b)NDBC model

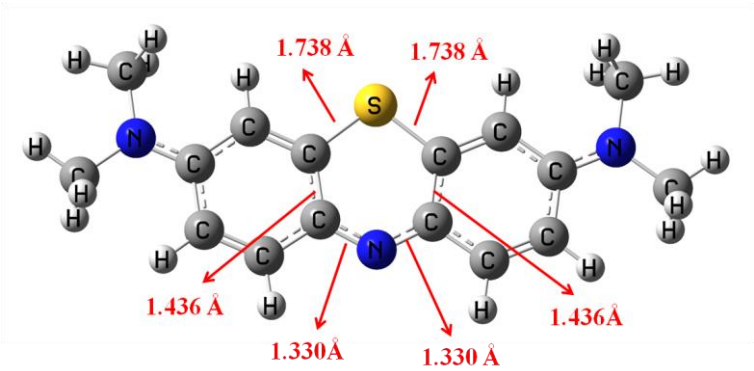


Fig. S2 Top-view of the optimized MB model

Table S1 QY of the NDBC

Sample	Emission intensity (I)	Abs at 320 nm (A)	Refractive index of solvent (n)	QY (%)
Quantum sulfate	4763842.857	0.042	1.33	55.7
NDBC	779149.1639	0.042	1.33	9.11

Table S2 Analysis of intermediate products of MB photodegradation by DBC

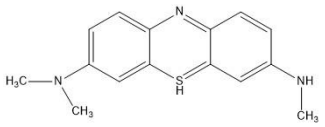
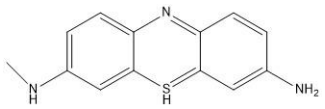
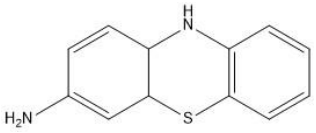
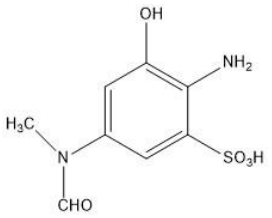
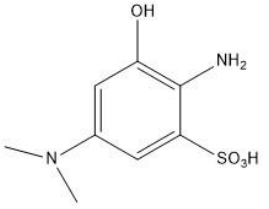
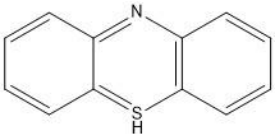
Products	Mass (m/z)	Molecular formula	Chemical structure
P1	270	$C_{15}H_{16}N_3S$	
P2	242	$C_{13}H_{14}N_3S$	
P3	217	$C_{12}H_{14}N_2S$	

Table S3 Analysis of intermediate products of MB photodegradation by NDBC

Product	Mass (m/z)	Molecular formula	Chemical structure
P1	246	$C_8H_{10}N_2O_5S$	
P2	232	$C_8H_{12}N_2O_4S$	
P3	202	$C_{12}H_9NS$	

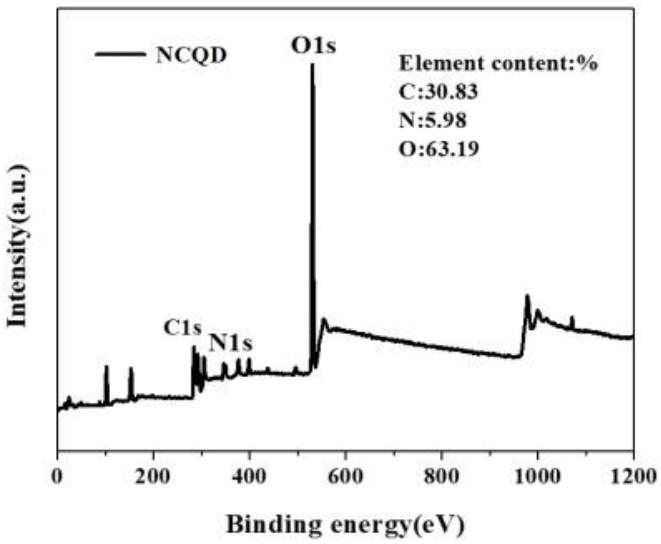


Fig. S3 Full XPS spectrum of NDBC

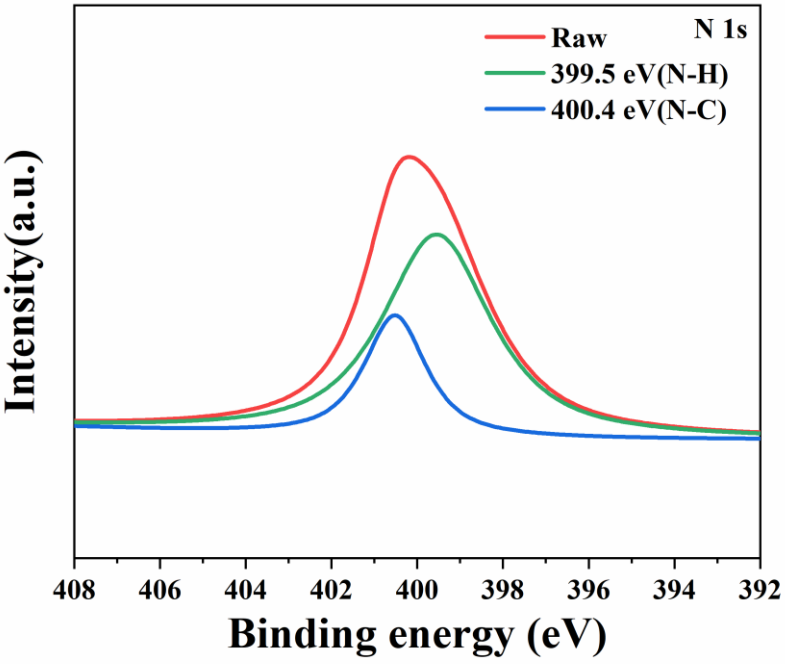


Fig. S4 N 1s XPS spectra and curve-fitting analysis of DBC

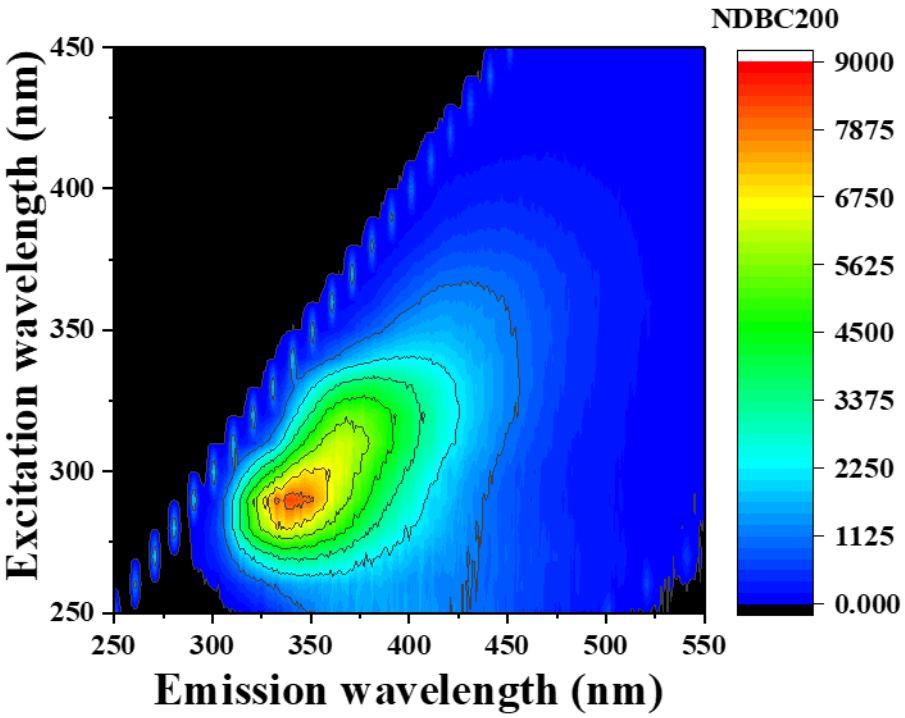


Fig. S5 EEM contours of NDBC200

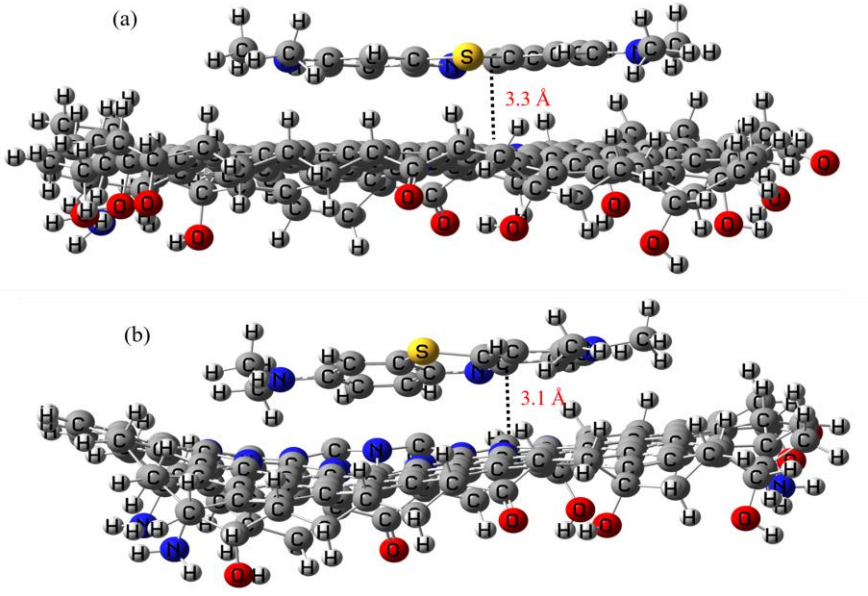


Fig. S6 (a) Side view of the optimized DBC-MB model; (b) side view of the optimized NDBC-MB model.

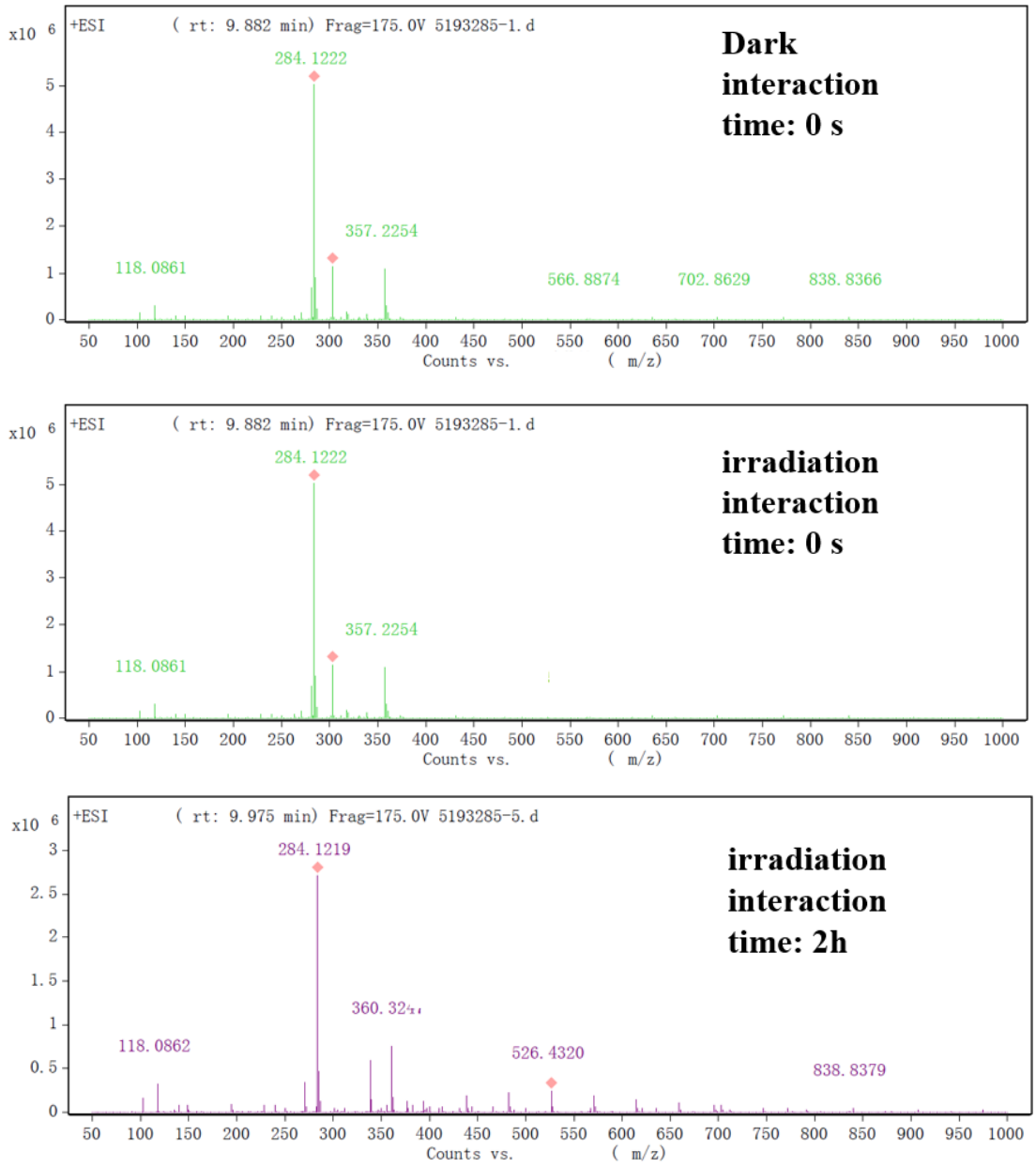


Fig. S7 HPLC-MS chromatogram of MB transformation intermediates in DBC with MB solution at different reaction times

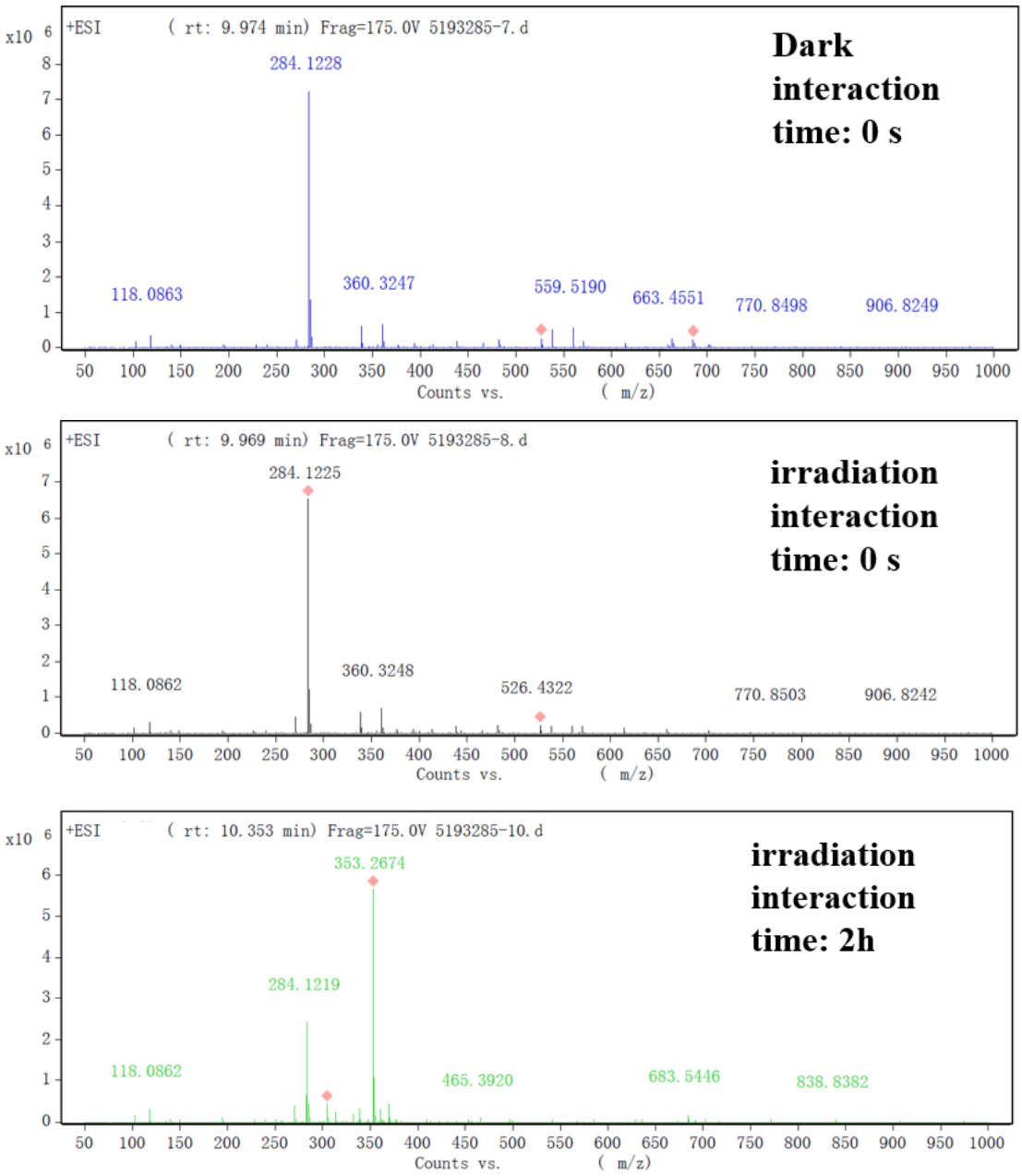


Fig. S8 HPLC-MS chromatogram of MB transformation intermediates in NDBC with MB solution at different reaction times

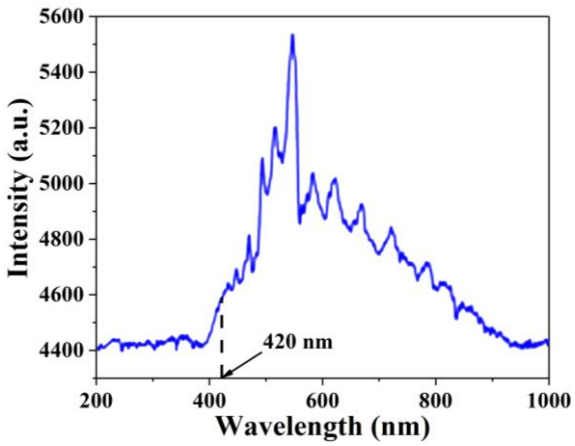


Fig. S9 Light spectrum of visible light source that used in the photodegradation experiments of TC and MB by NDBC under visible light irradiation. A 420 nm filter is used to remove the UV light that is emitted from the light source

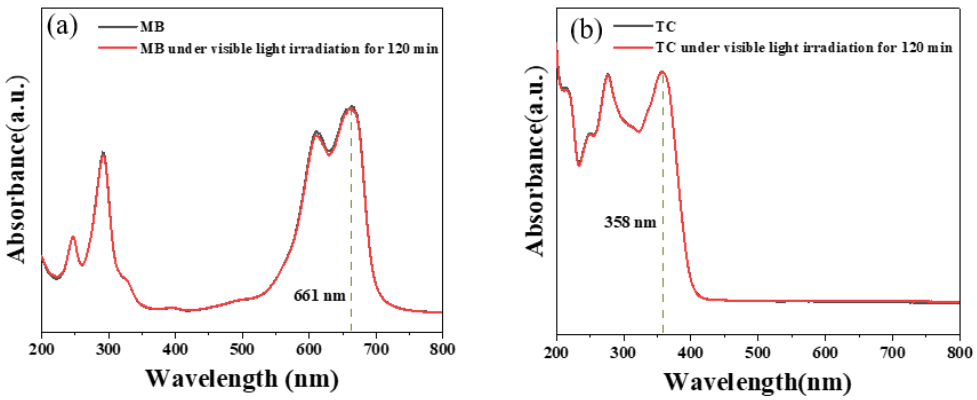


Fig. S10 (a) UV-Vis spectra of MB before and after visible light irradiation, in which the concentration of MB is 20 mg/L; (b) UV-Vis spectra of TC before and after visible light irradiation, in which the concentration of TC is 20 mg/L

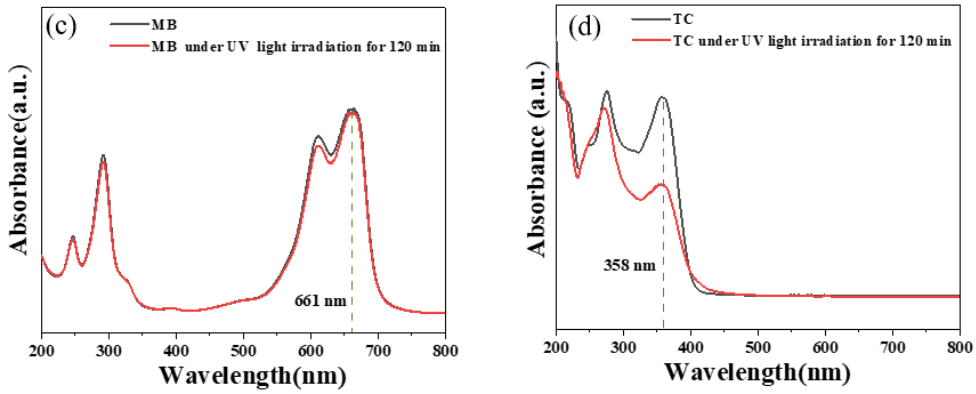


Fig. S11 (a) UV-Vis spectra of MB before and after UV light irradiation , in which the concentration of MB is 20 mg/L; (b) UV-Vis spectra of TC before and after UV light irradiation, in which the concentration of TC is 20 mg/L

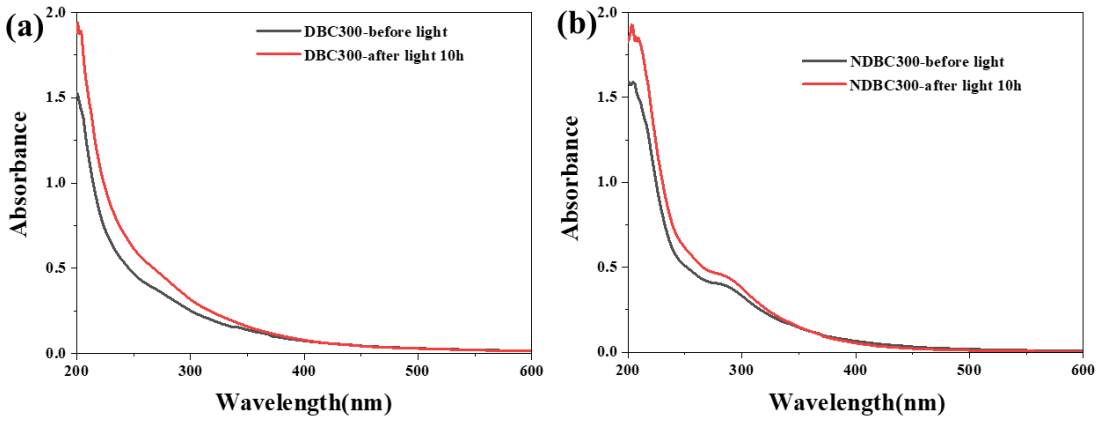


Fig. S12 UV-Vis spectra of (a) DBC300, and (b) NDBC300 before/after light irradiation 10 h

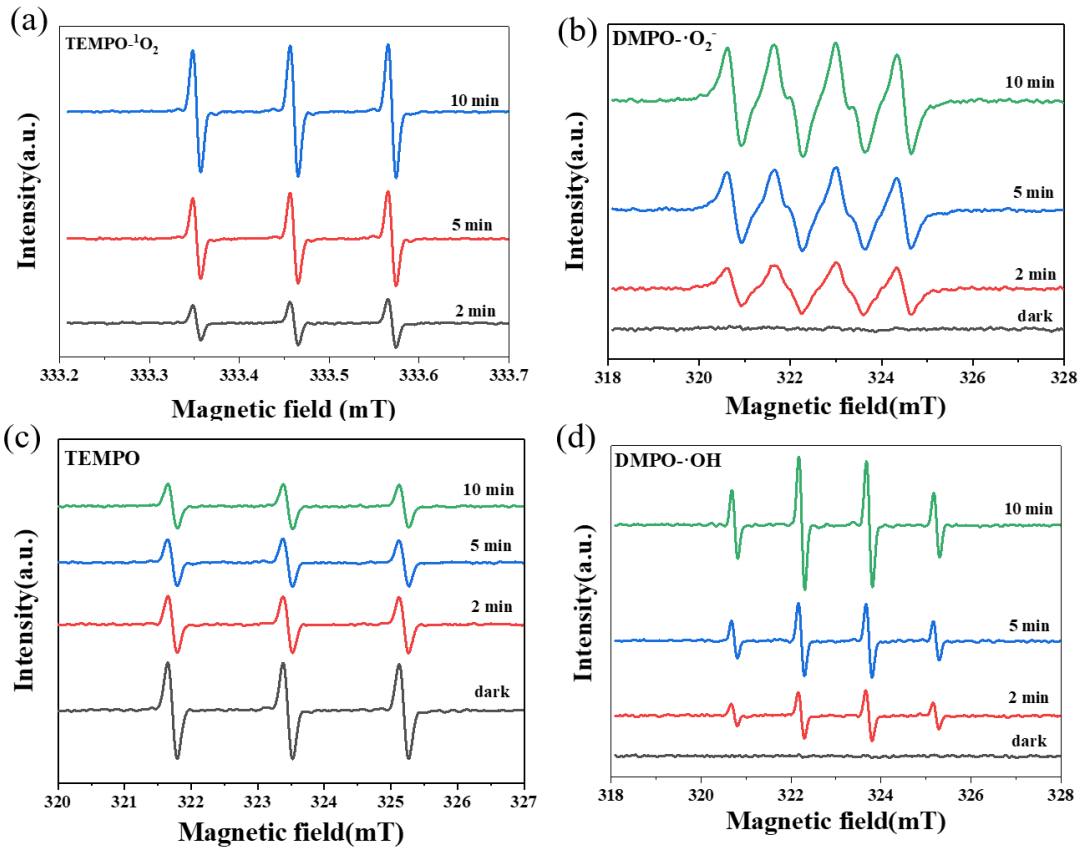


Fig. S13 EPR spectra of (a) DMPO-$^1O_2$; (b) DMPO- O_2^-; (c) TEMPO; (d) DMPO- OH

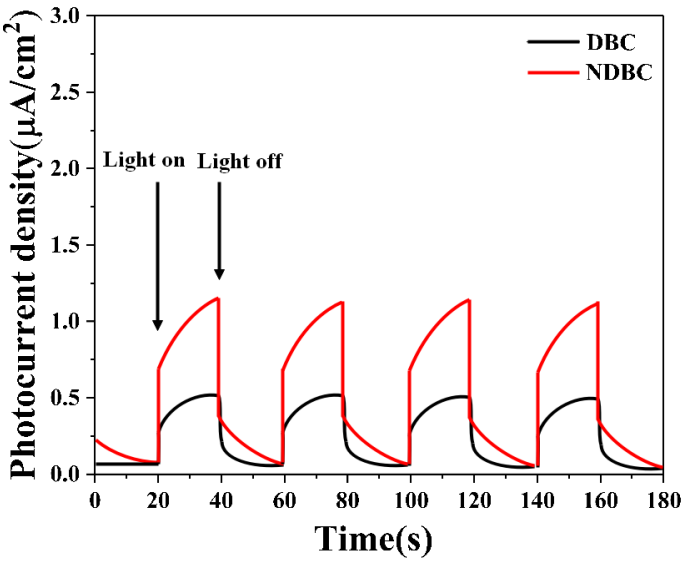
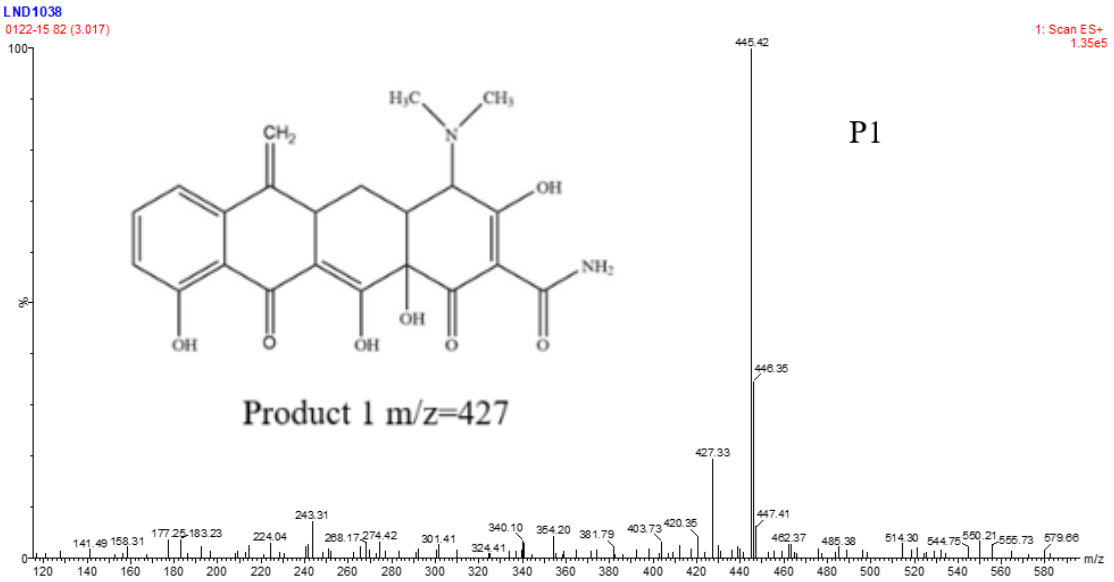


Fig. S14 Transient photocurrent response of NDBC and DBC composites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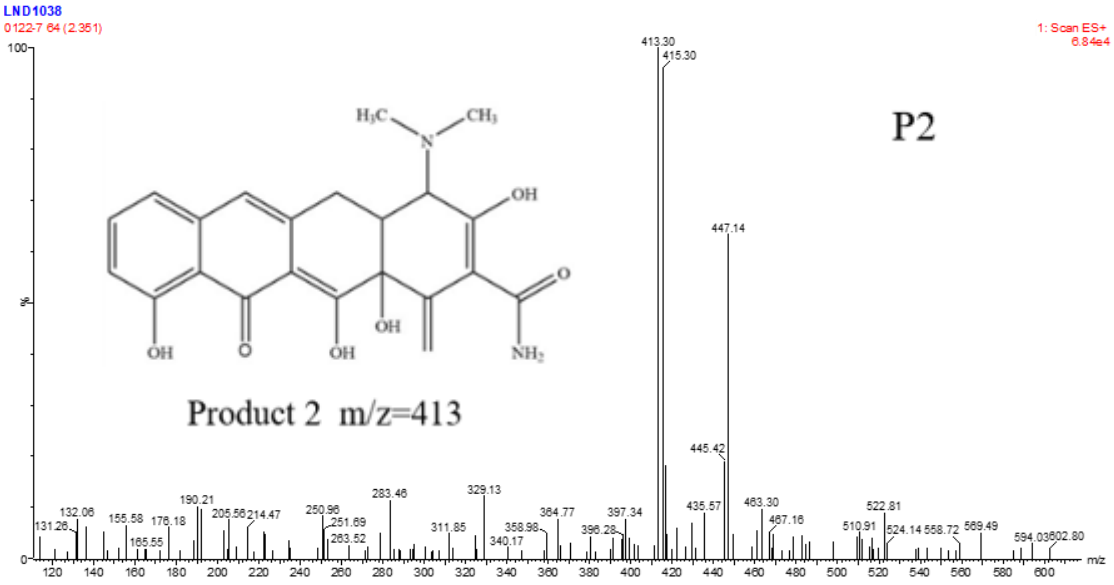
m/z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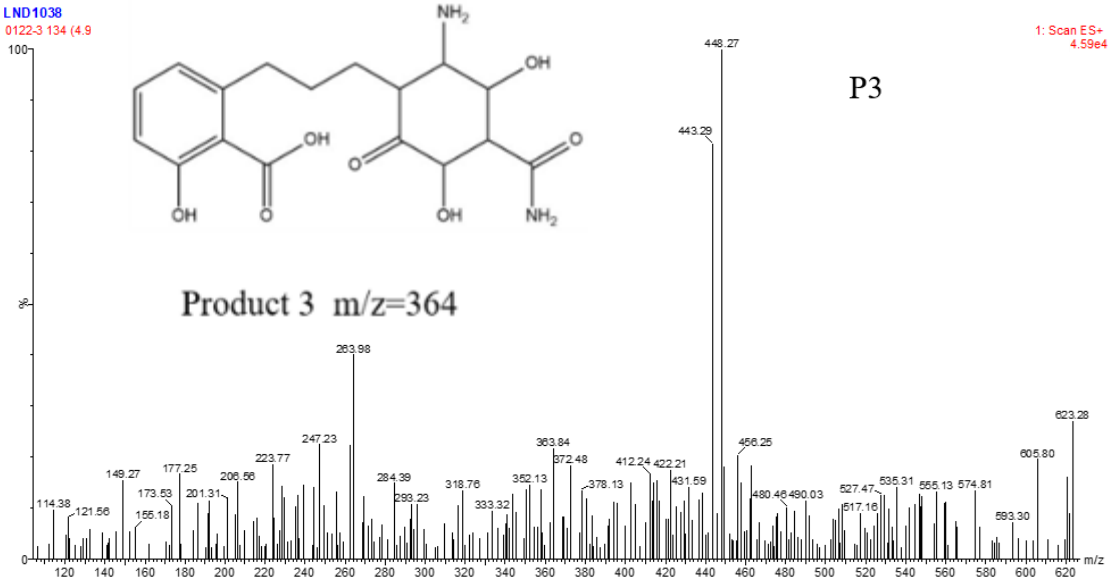
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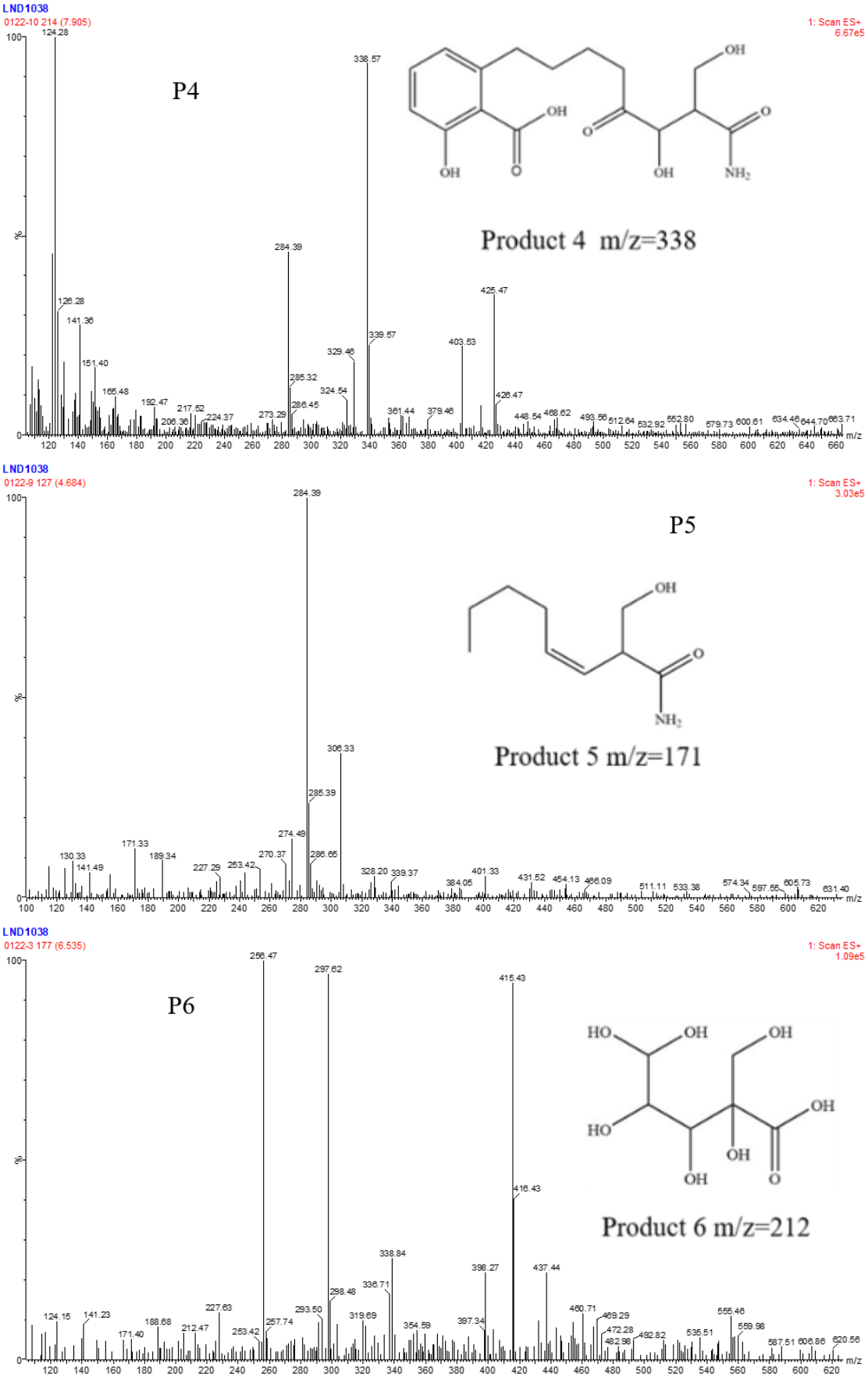

Fig. S15 HPLC-MS chromatogram of TC transformation intermediates in TC solution at different reaction time