

Supporting Information

Accelerated Indirect Photolysis of UV-328 within the Hydrophobic Microdomains of Dissolved Organic Matter: The Role of Sorption and Localized Reactive Intermediates

¹Mingzhu He^a, ¹Zhansheng Li^a, Hongxia Zhao^{a,*}, Yuhong Su^{b,*}, Shafiu Azam^a,
Jiawen Shao^a

^a Key Laboratory of Industrial Ecology and Environmental Engineering (Ministry of Education), School of Environmental Science and Technology, Dalian University of Technology, Dalian, 116024, China

^b College of Chemical Engineering, Petroleum and Natural Gas and Fine Chemicals Key Laboratory, Xinjiang University, Urumqi 830046, China

*Corresponding author.

Email: hxzhaodlut@dlut.edu.cn (H. Zhao), 194866912@qq.com (Y. Su).

Text S1. Materials and chemicals

2-(2H-benzotriazol-2-yl)-4,6-di-tert-amylphenol (UV-328) was produced by Sigma-Aldrich (Germany). Six DOM types were used in the experiment. Humic acid (HA) and fulvic acid (FA) were purchased from Sigma-Aldrich (St. Louis, MO, USA). The other four types of DOM were purchased from the International Humic Substances Association (IHSS), including Suwannee River natural organic matter (SRNOM, 2R101N), fulvic acid (SRFA, 3S101F), Mississippi River natural organic matter (MRNOM, 1R110N), and Leonardite humic acid (LHA, 1S104H). Ultrapure water was prepared using the Milli-Q Water Purification System ($\geq 18.2 \text{ M}\Omega\cdot\text{cm}$, Millipore, Bedford, USA). Chromatographic-grade dichloromethane, acetonitrile, and methanol were purchased from Sigma-Aldrich (Germany). Benzoic acid (BA), p-hydroxybenzoic Acid (p-HBA), 2,4,6-trimethylphenol (TMP), furfuryl alcohol (FFA), furfuryl alcohol derivative (furfurylamine, FFAm) were purchased from Aladdin Chemical Co., Ltd. (Shanghai, China). Sodium hydrogen phosphate, sodium dihydrogen phosphate, sodium hydroxide, and ammonium acetate were also purchased from Aladdin Chemical Co., Ltd. (Shanghai, China).

Text S2. Experimental details of solubility enhancement

The adsorption kinetics experiments of UV-328 and HA (10 and 20 mg C L⁻¹) were carried out for 6 days using the same experimental process as the solubility enhancement method. The reaction flask was kept in the dark at 25 °C, and three samples were collected repeatedly at each time point. Fig. S1 shows that it took at least 4 days to ensure that equilibrium was reached. Due to the high hydrophobicity of UV-328, the solubility enhancement data showed a high degree of dispersion. The concentration of the compound in each reaction flask far exceeded the water solubility

of the compound, so an important source of deviation from the data point was that UV-328 detached from the container wall during the equilibrium process. To reduce the deviation of the data, outliers were removed only when they exceeded ± 2 standard deviations from the mean of replicate measurements. Three replicate samples were prepared for each DOC concentration, and at least seven DOC concentrations were used to determine each K_{DOC} value. All replicate measurements for a single DOC concentration were excluded only when the mean significantly deviated from the 95% confidence interval.

Text S3. Study on spectral characteristics of DOM

Molar absorptivity at 280 nm (ϵ_{280}) was calculated as the UV absorbance at 280 nm normalized to the DOC concentration in mol C/L(1). The specific ultraviolet absorbance was calculated at 254 nm (SUVA_{254}), which is the absorbance per unit of organic carbon content(2). The fluorescence index (FI), a complementary parameter to ϵ_{280} , was calculated as the ratio of emission intensity at 470 nm to that at 520 nm at a fixed excitation wavelength (λ_{ex}) of 370 nm(3); the humification index (HIX) was calculated at $\lambda_{\text{ex}} = 254$ nm, dividing the total fluorescence over λ_{em} (emission wavelengths) = 435-480 nm by the total sum of fluorescence from $\lambda_{\text{em}} = 300-345$ nm and 435-480 nm; the biological index (BIX) was calculated at $\lambda_{\text{ex}} = 310$ nm as the ratio of fluorescence at $\lambda_{\text{em}} = 380$ nm to 430 nm(4).

Text S4. Photolysis contribution rate of PPRIs

$$k = k_{hv} + k_{\cdot OH} + k_{1O_2} + k_{3_{DOM}^*} + k_{others} \#S4.1$$

The calculation formula for $\cdot OH$ contribution rate:

$$\cdot OH\% = \frac{k_{\cdot OH}}{k} = 1 - \frac{k_{IPA}}{k} \quad \#S4.2$$

The calculation formula of $^3DOM^*$ contribution rate:

$$^3DOM^*\% = \frac{k_{^3DOM^*}}{k} = 1 - \frac{k_{TMP}}{k} - \frac{k_{IPA} - k_{NaN_3}}{k} \quad \#S4.3$$

The calculation formula of 1O_2 contribution rate:

$$^1O_2\% = \frac{k_{^1O_2}}{k} = 1 - \frac{k_{NaN_3}}{k} - \left(1 - \frac{k_{IPA}}{k}\right) = \frac{k_{IPA}}{k} - \frac{k_{NaN_3}}{k} \quad \#S4.4$$

In these equations, k was the total photodegradation rate constant of UV-328; $k_{\cdot OH}$ was the reaction rate constant of $\cdot OH$ and UV-328; $k_{^1O_2}$ was the reaction rate constant of 1O_2 and UV-328; $k_{^3DOM^*}$ was the reaction rate constant of $^3DOM^*$ and UV-328. The k_{IPA} , k_{TMP} , and k_{NaN_3} were the reaction rate constant after adding quenchers IPA, TMP, and NaN_3 , respectively.

Text S5. Determination of the second-order reaction rate constant of UV-328 and PPRI

S5.1. The second-order reaction rate constant of UV-328 with $\cdot OH$ ($k_{UV-328, \cdot OH}$)

$\cdot OH$ was generated by the UV/ H_2O_2 system. The second-order reaction rate constant of UV-328 with $\cdot OH$ was determined by competition kinetics using BA as a probe. Given the pKa of BA (≈ 4.2), BA exists predominantly as deprotonated benzoate ion (BzO^-) under our experimental neutral pH conditions. Therefore, $k_{BzO^-, \cdot OH}$ ($5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$) was the second-order reaction rate constant for the reaction of BzO^- and $\cdot OH$ (5). The concentrations of H_2O_2 , UV-328, and BA in the reaction system were 5

mM, 5 μ M, and 5 μ M. 1 mL aliquots were taken at predetermined time intervals, and the residual H_2O_2 was immediately quenched with 20 μ L of 1.0 M $\text{Na}_2\text{S}_2\text{O}_3$. The second-order rate constant $k_{UV-328,OH}$ was calculated using the following equation:

$$k_{UV-328,OH} = \frac{\ln\left(\frac{[UV-328]_t}{[UV-328]_0}\right)}{\ln\left(\frac{[BA]_t}{[BA]_0}\right)} k_{B_2O_2^-,OH} \quad \#S5.1$$

S5.2. The second-order reaction rate constant of UV-328 with $^1\text{O}_2$ ($k_{UV-328,^1O_2}$)

In the molybdate/ H_2O_2 catalytic system, molybdate catalyzed the disproportionation reaction of H_2O_2 to produce $^1\text{O}_2$. FFA, which had a known second-order reaction rate constant with $^1\text{O}_2$, was used as a probe to determine $k_{UV-328,^1O_2}$ by competitive kinetics. The concentrations of MnO_4^{2-} , H_2O_2 , UV-328 and FFA were 1 mM, 10 mM, 5 μ M, respectively. At predetermined time intervals, 1 mL aliquots were transferred to a vial pre-filled with 50 μ L of 10 mM histidine to quench the residual $^1\text{O}_2$. The second-order rate constant $k_{UV-328,^1O_2}$ was calculated using the following equation:

$$k_{UV-328,^1O_2} = \frac{\ln\left(\frac{[UV-328]_t}{[UV-328]_0}\right)}{\ln\left(\frac{[FFA]_t}{[FFA]_0}\right)} k_{FFA,^1O_2} \quad \#S5.2$$

S5.3. The second-order reaction rate constant of UV-328 with $^3\text{RB}^*$ ($k_{UV-328,^3\text{RB}^*}$)

$^3\text{DOM}^*$ is an important reactive intermediate in natural water. However, due to the complex structure and large molecular weight of $^3\text{DOM}^*$, it was difficult to directly determine. Therefore, small-molecular-weight compounds with quinone and ketone chromophores were often used as model compounds. The commonly used small molecular model compounds were riboflavin (RB), sodium anthraquinone-2-sulfonate (AQ2S), 1-nitronaphthalene, etc. Compared with $^3\text{AQ2S}^*$, the energy levels and redox

potentials of ${}^3\text{RB}^*$ are closer to those of ${}^3\text{DOM}^*$ (6). Therefore, in this study, RB was used as a small-molecule model compound for DOM to determine the second-order reaction rate constant for ${}^3\text{RB}^*$ with UV-328.

RB was excited to ${}^3\text{RB}^*$ upon light absorption. ${}^3\text{RB}^*$ can react with UV-328 and also generate ${}^1\text{O}_2$ via energy transfer. Therefore, it is necessary to consider the simultaneous reactions of UV-328 with both ${}^1\text{O}_2$ and ${}^3\text{RB}^*$. The reaction scheme is as follows:

$$R_{3\text{RB}^*} = \sum_{\lambda} \frac{I_{\lambda} \varepsilon_{\lambda}^{\text{RB}} (1 - 10^{-\varepsilon_{\lambda}^{\text{RB}} [\text{RB}] l})}{\varepsilon_{\lambda}^{\text{RB}} [\text{RB}] l} [\text{RB}] \Phi_{3\text{RB}^*} \quad \#55.3$$

Here, $R_{3\text{RB}^*}$ was the formation rate of ${}^3\text{RB}^*$ (M s^{-1}); $[\text{RB}]$ was the initial concentration of RB (M); $\varepsilon_{\lambda}^{\text{RB}}$ was the molar absorption coefficient of RB at the wavelength of λ nm ($\text{cm}^{-1} \text{M}^{-1}$). $\Phi_{3\text{RB}^*}$ was the quantum yield of ${}^3\text{RB}^*$ excited by RB after light absorption, which was 0.375(7); I_{λ} was the light intensity at the center of the quartz tube ($\text{einstein cm}^{-2} \text{s}^{-1}$) under the irradiation of a 500 W mercury lamp with a 290 nm filter. The measured value of I_{λ} was 3×10^{-5} using a chemical actinometer.

$$R_{\text{UV}-328} = R_{3\text{RB}^*} \left(\frac{k_{\text{UV}-328, 3\text{RB}^*} \cdot [\text{UV}-328]}{4.2 \times 10^5 + k_{\text{UV}-328, 3\text{RB}^*} \cdot [\text{UV}]} \right) \quad \#55.4$$

Here, $R_{\text{UV}-328}$ is the initial degradation rate constant of UV-328 ($\text{M}^{-1} \text{s}^{-1}$); $4.2 \times 10^5 \text{ s}^{-1}$ is the quenching rate constant of ${}^3\text{RB}^*$ under aerobic conditions; $1.5 \times 10^5 \text{ s}^{-1}$ is the quenching rate of ${}^3\text{RB}^*$ under anaerobic conditions. The difference between them represents the quenching rate constant for the reaction of ${}^3\text{RB}^*$ with ground-state O_2

$(2.7 \times 10^5 \text{ s}^{-1})$. $2.5 \times 10^5 \text{ s}^{-1}$ is the thermal inactivation rate of $^1\text{O}_2$ (8).

Text S6. Molecular probe experiment

S6.1. $\cdot\text{OH}$

BA was used as a molecular probe to determine the steady-state concentration of $\cdot\text{OH}$ ($[\cdot\text{OH}]_{ss}$) in the reaction system by measuring the rate at which BA reacted with $\cdot\text{OH}$ to form p-hydroxybenzoic acid (p-HBA). BA was added to a 10 mg C L^{-1} DOM solution at an initial concentration of 0.5 mM . After a period of illumination, samples were taken at regular intervals and passed through a $0.22 \mu\text{m}$ nylon membrane filter for HPLC analysis. The formation rate of p-HBA (R_{p-HBA}) and the formation rate of $\cdot\text{OH}$ ($R_{\cdot\text{OH}}$) were obtained from the following equation, and the conversion factor between them was $5.87 \pm 0.18(9)$.

$$R_{\cdot\text{OH}} = R_{p-HBA} \cdot 5.87 \quad \#S6.1$$

$[\cdot\text{OH}]_{ss}$ was calculated using the following equation:

$$[\cdot\text{OH}]_{ss} = \frac{R_{\cdot\text{OH}}}{k_{BzO^-, \cdot\text{OH}} \cdot [\text{BA}]} \quad \#S6.2$$

Here, $[\text{BA}]$ was the initial concentration of benzoic acid (M).

S6.2. $^3\text{DOM}^*$

The steady-state concentration of $^3\text{DOM}^*$ ($[^3\text{DOM}^*]_{ss}$) was determined using TMP as the probe molecule. TMP was added to a 10 mg C L^{-1} DOM solution at an initial concentration of $100 \mu\text{M}$. After regular sampling, the samples were passed through a $0.22 \mu\text{m}$ glass fiber filter for HPLC analysis. Although TMP can also react with $^1\text{O}_2$ and $\cdot\text{OH}$, the contribution of $^1\text{O}_2$ and $\cdot\text{OH}$ to TMP conversion was negligible(10, 11).

The formation rate of ${}^3\text{DOM}^*$ ($R_{{}^3\text{DOM}^*}$) could be obtained from the following equation:

$$R_{{}^3\text{DOM}^*} = R_{\text{TMP}} \cdot \frac{S_{{}^3\text{DOM}^*} + k_{\text{TMP}, {}^3\text{DOM}^*} \cdot [\text{TMP}]}{k_{\text{TMP}, {}^3\text{DOM}^*} \cdot [\text{TMP}]} \quad \#S6.3$$

Here, $[\text{TMP}]$ was the initial concentration of TMP (M), R_{TMP} was the initial degradation rate of TMP (M s^{-1}), $k_{\text{TMP}, {}^3\text{DOM}^*}$ was the second-order reaction rate constant for the reaction of TMP and ${}^3\text{DOM}^*$ ($8.1 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$), $S_{{}^3\text{DOM}^*}$ ($3.1 \times 10^5 \text{ s}^{-1}$) was the sum of the rate constant for the reaction of ${}^3\text{DOM}^*$ with ground-state dissolved oxygen ($2.2 \times 10^5 \text{ s}^{-1}$) and the quenching rate constant of ${}^3\text{DOM}^*$ ($9.0 \times 10^4 \text{ s}^{-1}$) caused by other factors(12).

$[{}^3\text{DOM}^*]_{\text{ss}}$ was calculated using the following equation:

$$[{}^3\text{DOM}^*]_{\text{ss}} = \frac{R_{{}^3\text{DOM}^*}}{S_{{}^3\text{DOM}^*} + k_{\text{TMP}, {}^3\text{DOM}^*} \cdot [\text{TMP}]} \quad \#S6.4$$

S6.3. ${}^1\text{O}_2$

The results of Cheng et al(13) showed that in the pH range of 4-8, due to an increase in the proportion of deprotonated carboxylic acid and phenolic groups, the charge density of DOM increased. The deprotonation of these groups led to an increase in the surface potential of DOM, which attracted more FFAm to accumulate near DOM, and the concentration of FFAm near DOM gradually increased. However, when the pH was further increased to 8-9, the proportion of neutral FFAm increased, resulting in a decrease in FFAm concentration near DOM. Therefore, in order to accumulate more FFAm near the DOM, the pH was maintained at 8 in this experiment. FFA and FFAm were dissolved in water to prepare a 50 mM stock solution. A 100 mM buffer salt solution with pH=8 was prepared using sodium dihydrogen phosphate and disodium

hydrogen phosphate. A 10 mg C L⁻¹ DOM solution was prepared in 10 mM phosphate buffer, containing 100 μM FFA or FFAm. After regular sampling, the samples were passed through a 0.22 μm glass fiber filter for HPLC analysis. The apparent concentration of ¹O₂ ($[^1O_2]_{app}$) measured by FFA and FFAm was calculated using the following equation:

$$[^1O_2]_{app}^{FFA} = \frac{k_{obs}^{FFA}}{k_{rxn}^{FFA}} \quad \#S6.5$$

$$[^1O_2]_{app}^{FFAm} = \frac{k_{obs}^{FFAm}}{k_{rxn}^{FFAm}} \quad \#S6.6$$

Here, k_{obs}^{FFA} and k_{obs}^{FFAm} were the photolysis rate constants of FFA and FFAm (s⁻¹), k_{rxn}^{FFA} was the second-order reaction rate constant for the reaction of FFA and ¹O₂ (1.0 × 10⁸ M⁻¹ s⁻¹)(14), and k_{rxn}^{FFAm} was the second-order reaction rate constant of FFAm and ¹O₂, which was calculated using the following equation:

$$k_{rxn}^{FFAm} = \frac{1}{1 + 10^{(pH - pKa)}} \cdot k_{rxn}^{FFAm^+} + \frac{10^{(pH - pKa)}}{1 + 10^{(pH - pKa)}} \cdot k_{rxn}^{FFAm^0} \quad \#S6.7$$

Here, pKa was the dissociation constant of FFAm (9.01 ± 0.07), $k_{rxn}^{FFAm^+}$ was the second-order reaction rate constant for the reaction of $FFAm^+$ with ¹O₂ (4.32 × 10⁷ M⁻¹ s⁻¹), and $k_{rxn}^{FFAm^0}$ was the second-order reaction rate constant for the reaction of $FFAm^0$ with ¹O₂ (2.07 × 10⁸ M⁻¹ s⁻¹)(13).

Text S7. Indirect photolysis rate constants induced by free and bound PPRIs

When DOM and UV-328 coexist in the reaction system, competitive light absorption occurs between them, and inhibiting direct photolysis of the target. The

direct photolysis rate constant of the target in the DOM solution can be corrected using the light screening factor S_λ . S_λ can be calculated using the following equation(15):

$$S_\lambda = \frac{(1 - 10^{-\alpha_\lambda \times l})}{2.303 \times \alpha_\lambda \times l} \#S7.1$$

Here, α_λ (cm^{-1}) was the beam attenuation coefficient (the absorbance of DOM at wavelength λ with a 1 cm path length); l (cm) was the optical path of the quartz photolysis tube receiving light, and which was 2.3 cm in this study. α_λ could be obtained by measuring the absorbance (A) of the corresponding wavelength (λ m) at the wavelength of maximum specific light absorption (I_λ^{abs}). The calculation method of I_λ^{abs} was as follows: $2.3 \times$ light intensity at a specific wavelength \times molar absorption coefficient at a specific wavelength(16). Since the measured light intensities were relative, only the relative I_λ^{abs} (I_λ^{abs}) was calculated. As shown in Fig. S8, the wavelength maximum λ_m corresponding to I_λ^{abs} was 297 nm. The screening coefficient S_λ was calculated by using the absorbance of DOM at this wavelength.

Based on S_λ for DOM-UV-328 solutions, the indirect photodegradation rate constant k_{ind} of UV-328 initiated by DOM can be calculated(17):

$$k_{ind} = k_{obs(with - DOM)} - k_d \times S_\lambda \#S7.2$$

In the equation, $k_{obs(with - DOM)}$ was the apparent photodegradation rate constant (h^{-1}) of UV-328 in the DOM solution, and k_d was the direct photodegradation rate constant of UV-328. k_{ind} can also be expressed as follows:

$$k_{ind} = k_{UV-328,OH}[\cdot OH]_{free,ss} + k_{UV-328,OH}[\cdot OH]_l S7.3 \\ + [^1O_2]_{bonded,ss} + k_{UV-328,^3RB^*} [^3DOM^*]_{free,ss}$$

Here, $[RIS]_{free,ss}$ was the steady-state concentration of free PPRIs, $[RIS]_{bonded,ss}$ was the steady-state concentration of bound PPRIs, $k_{UV-328,OH}$, $k_{UV-328,^1O_2}$, and $k_{UV-328,^3RB^*}$ were the second-order reaction rate constants for the reactions of UV-328 with PPRIs.

Text S8. Analysis method

The quantification of pollutants and other substances was performed by high-performance liquid chromatography (HPLC, Shimadzu, Japan). The SB-C18 chromatographic column (particle size 5 μ m, 2.1 mm \times 150 mm, Agilent, USA) was selected. The chromatographic conditions are summarized in Table S2.

UV-328 and its photoconversion products were determined by high-performance liquid chromatography–tandem mass spectrometry (HPLC-MS/MS, Q Exactive Plus, USA). Electrospray ionization (ESI) was performed in positive ion mode, and the mass scan range was 60-1000 Da. In the experiment, the Hypersil GOLD C18 column was used as the chromatographic column, and its specification was 150 mm long, 2.1 mm inner diameter, and the filling particle size was 3 μ m. The mobile phase consisted of ultrapure water and methanol. The flow rate was controlled at 0.2 mL/min. The injection volume was 10 μ L. This ensured the accuracy and repeatability of the analysis. A gradient elution procedure was used to achieve effective separation of different components. From 0 to 20 min, the methanol percentage gradually increased from 0% to 80%, and then the proportion of methanol was maintained at 5% for 20-25 min to

further optimize the separation effect. In the next critical stage, the methanol ratio increased rapidly from 5% to 80%, covering 25 to 26 min to achieve complete elution of the target compounds. In the last 25-35 min, the methanol ratio was maintained at 80%, to ensure complete elution and obtain clean chromatograms for subsequent analysis. Through such a gradient elution strategy, various components in the sample were effectively separated and identified. Data acquisition and processing were performed using Xcalibur software.

Table S1. Brief information of pollutants

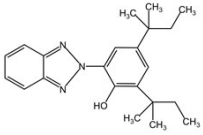
Compounds	Abbreviations	CAS	Structural formula	pKa	logKow
2-(2H-benzotriazol-2-yl)- 4,6-di-tert-amylphenol	UV-328	21615-49-6		8.59	7.25

Table S2. Analysis conditions of liquid chromatography

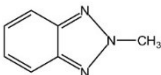
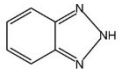
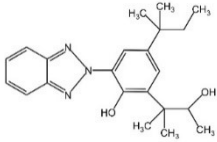
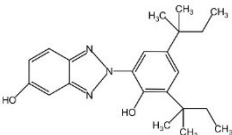
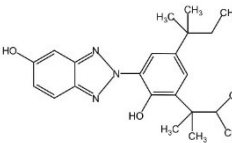
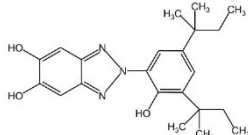
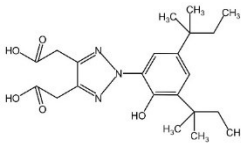
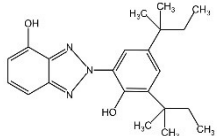
Name	Flow phase and proportion	Wavelength (nm)	Flow velocity (mL/min)	Sample marking size (μL)
UV-328	Water:Acetonitrile (0:100)	345	1.5	10
TMP	Water:Acetonitrile (40:60)	205	1.0	30
p-HBA	1% Acetic acid water:Methanol (40:60)	205	1.0	30
FFA	0.025 mM Ammonium acetate: Acetonitrile (75:25)	219	1.0	50
FFAm	0.025 mM Ammonium acetate: Acetonitrile (75:25)	219	1.0	50

Table S3. Calculated values of $k_{UV-328,RI_s}[RIS]_{ss}$ for UV-328 in different DOM solutions (aqueous phase and hydrophobic microdomain)

$k_{UV-328,RI_s}[RIS]_{ss}$	HA	FA	SRNOM
$k_{UV-328,OH[\cdot OH]}_{free,ss}$	$(4.37 \pm 0.20) \times 10^{-8}$	$(2.75 \pm 0.12) \times 10^{-8}$	$(2.22 \pm 0.16) \times 10^{-8}$
$k_{UV-328,OH[\cdot OH]}_{bonded,ss}$	$(4.37 \pm 0.20) \times 10^{-6}$	$(2.75 \pm 0.12) \times 10^{-6}$	$(2.22 \pm 0.16) \times 10^{-6}$
$k_{UV-328,^1O_2}[^1O_2]_{free,ss}$	$(2.02 \pm 0.11) \times 10^{-5}$	$(1.33 \pm 0.10) \times 10^{-5}$	$(0.71 \pm 0.34) \times 10^{-5}$
$k_{UV-328,^1O_2}[^1O_2]_{bonded,ss}$	$(2.02 \pm 0.11) \times 10^{-3}$	$(1.33 \pm 0.10) \times 10^{-3}$	$(0.71 \pm 0.34) \times 10^{-3}$
$k_{UV-328,^3RB^*}[^3DOM^*]_{free,ss}$	$(1.44 \pm 0.11) \times 10^{-4}$	$(8.34 \pm 0.66) \times 10^{-5}$	$(4.79 \pm 0.36) \times 10^{-5}$
$k_{UV-328,^3RB^*}[^3DOM^*]_{bonded}$	$(1.44 \pm 0.11) \times 10^{-2}$	$(8.34 \pm 0.66) \times 10^{-3}$	$(4.79 \pm 0.36) \times 10^{-3}$

Table S4. UV-328 photolysis product information

Products	RT (min)	Precise mass ((M+H) ⁺ m/z)	Measured mass ((M+H) ⁺ m/z)	Molecular formula	Structural formula
UV-328	12.90	352.2383	352.2399	C ₂₂ H ₂₉ N ₃ O	
P250	18.32	251.2005	251.2001	C ₁₆ H ₂₆ O ₂	
P353	13.49	354.2176	354.2144	C ₂₁ H ₂₇ N ₃ O ₂	
P281	17.66	282.1600	282.1591	C ₁₇ H ₁₉ N ₃ O	
P211	7.83	212.0818	212.0799	C ₁₂ H ₉ N ₃ O	

P133	1.56	134.0713	134.0711	$C_7H_7N_3$	
P119	4.39	120.0556	120.0554	$C_6H_5N_3$	
P367	3.61	368.2332	368.2302	$C_{22}H_{29}N_3O_2$	
	6.02	368.2332	368.2290		
P383	6.96	384.2281	384.2246	$C_{22}H_{29}N_3O_3$	
	8.96	384.2281	384.2318		
P417	14.23	418.2336	418.2311	$C_{22}H_{31}N_3O_5$	
P369	1.44	370.2489	370.2452	$C_{22}H_{31}N_3O_2$	

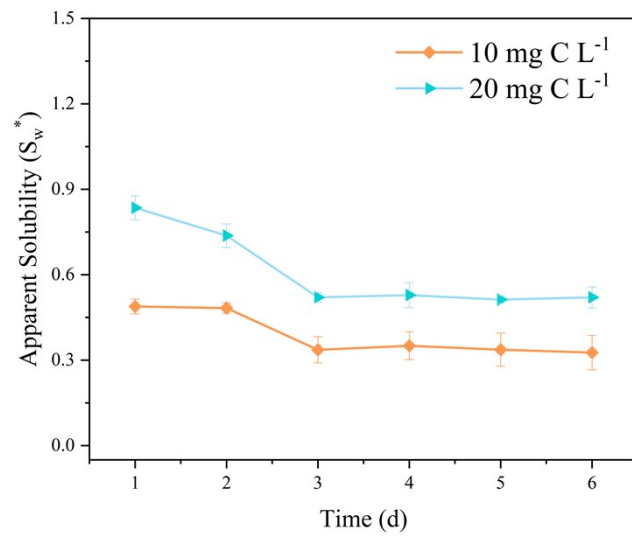


Fig. S1. Equilibrium Kinetics of UV-328 in HA-H₂O System.

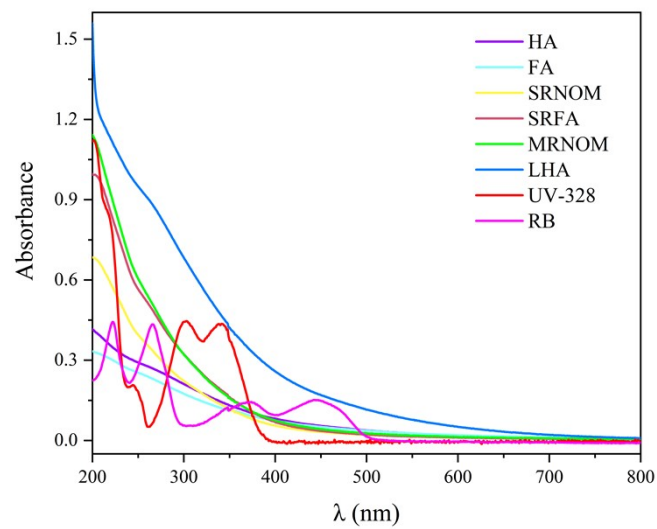


Fig. S2. UV-visible absorption spectra of UV-328 (spectra multiplied by a factor of 5 for clarity), DOM and RB.

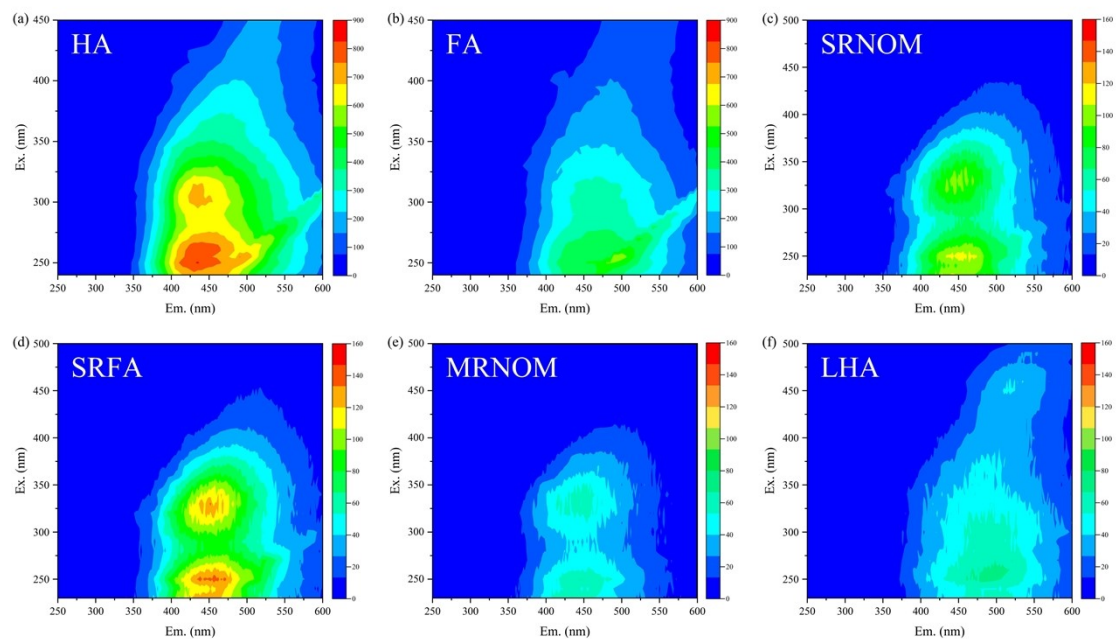


Fig. S3. Three-dimensional fluorescence spectra of DOM.

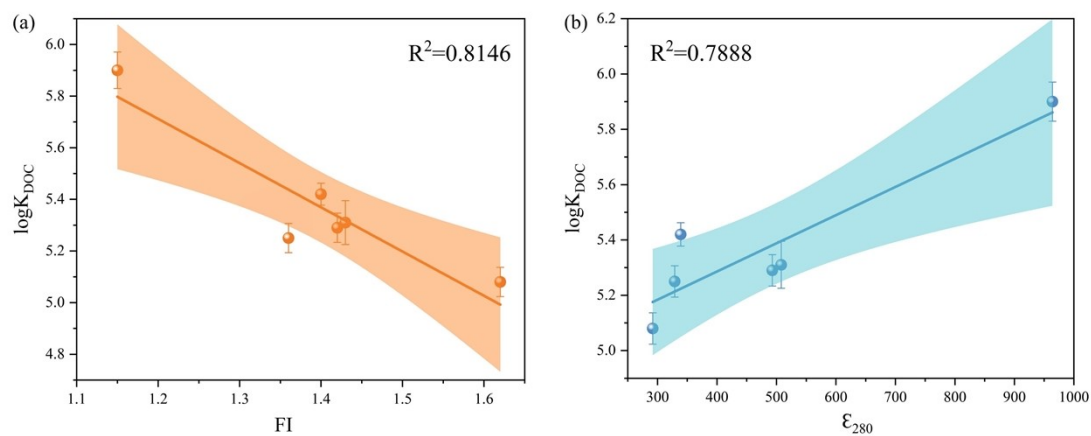


Fig. S4. The linear fitting of the measured value of $\log K_{\text{DOC}}$ with FI and ϵ_{280} .

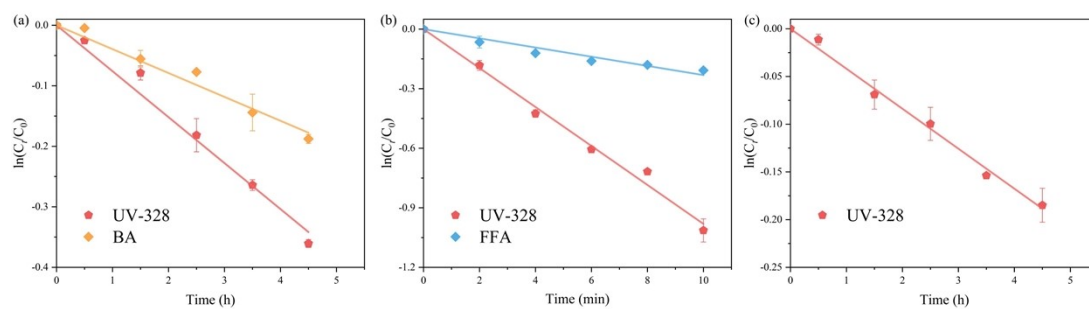


Fig. S5. (a) The second-order rate constant of UV-328 with $\cdot\text{OH}$ was determined by the competition kinetics method in the $\text{H}_2\text{O}_2/\text{UV}$ system; (b) Molybdate/ H_2O_2 catalytic system produced $^1\text{O}_2$, and the second-order rate constant for the reaction of UV-328 and $^1\text{O}_2$ was determined using competition kinetics; (c) The second-order rate constants of UV-328 and $^3\text{RB}^*$ were determined using RB as a DOM model compound.

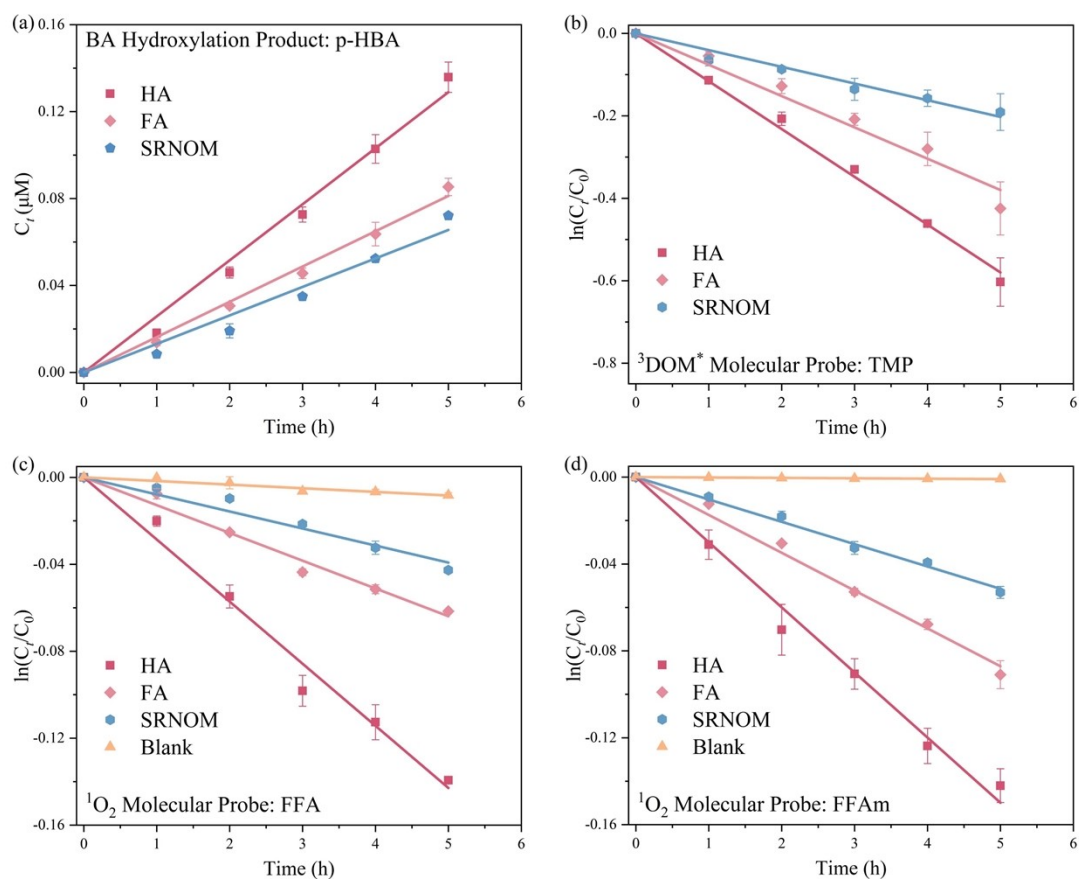


Fig. S6. (a) BA was used as a probe to determine the steady-state concentration of $\cdot\text{OH}$; (b) TMP was used as a probe to measure the steady-state concentration of $^3\text{DOM}^*$; (c) FFA was used as a probe to determine the steady-state concentration of $^1\text{O}_2$; (d) FFAm was used as a probe to determine the steady-state concentration of $^1\text{O}_2$. (DOM concentration: 10 mg C L^{-1} .)

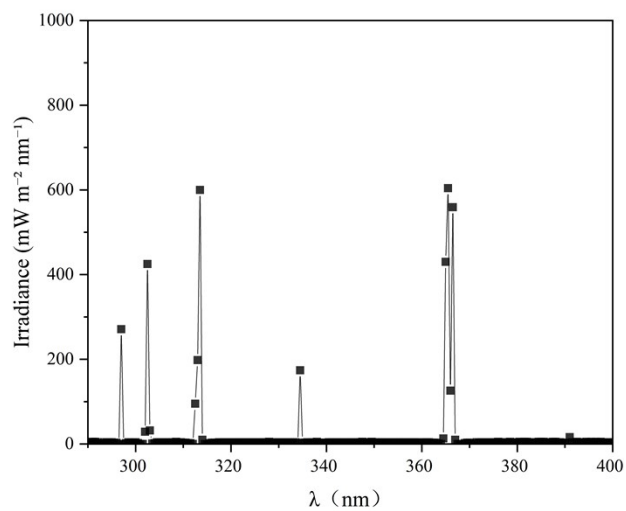


Fig. S7. Emission spectrum of the mercury lamp used in the photolysis experiments, recorded over the wavelength range 290-400 nm.

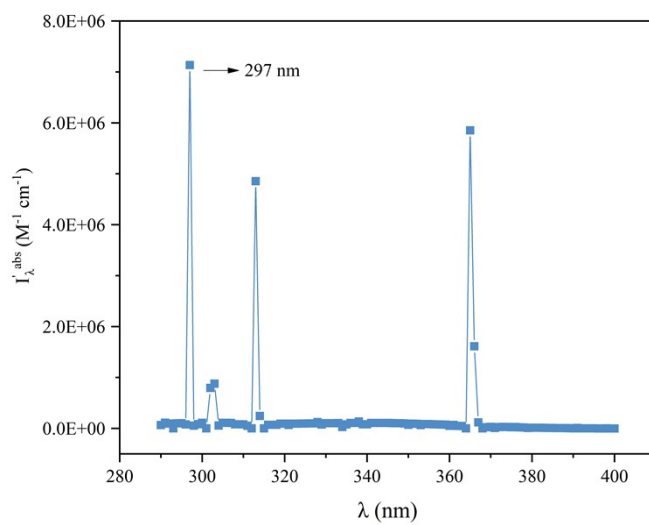


Fig. S8. Relative specific light absorption rate of UV-328 in water.

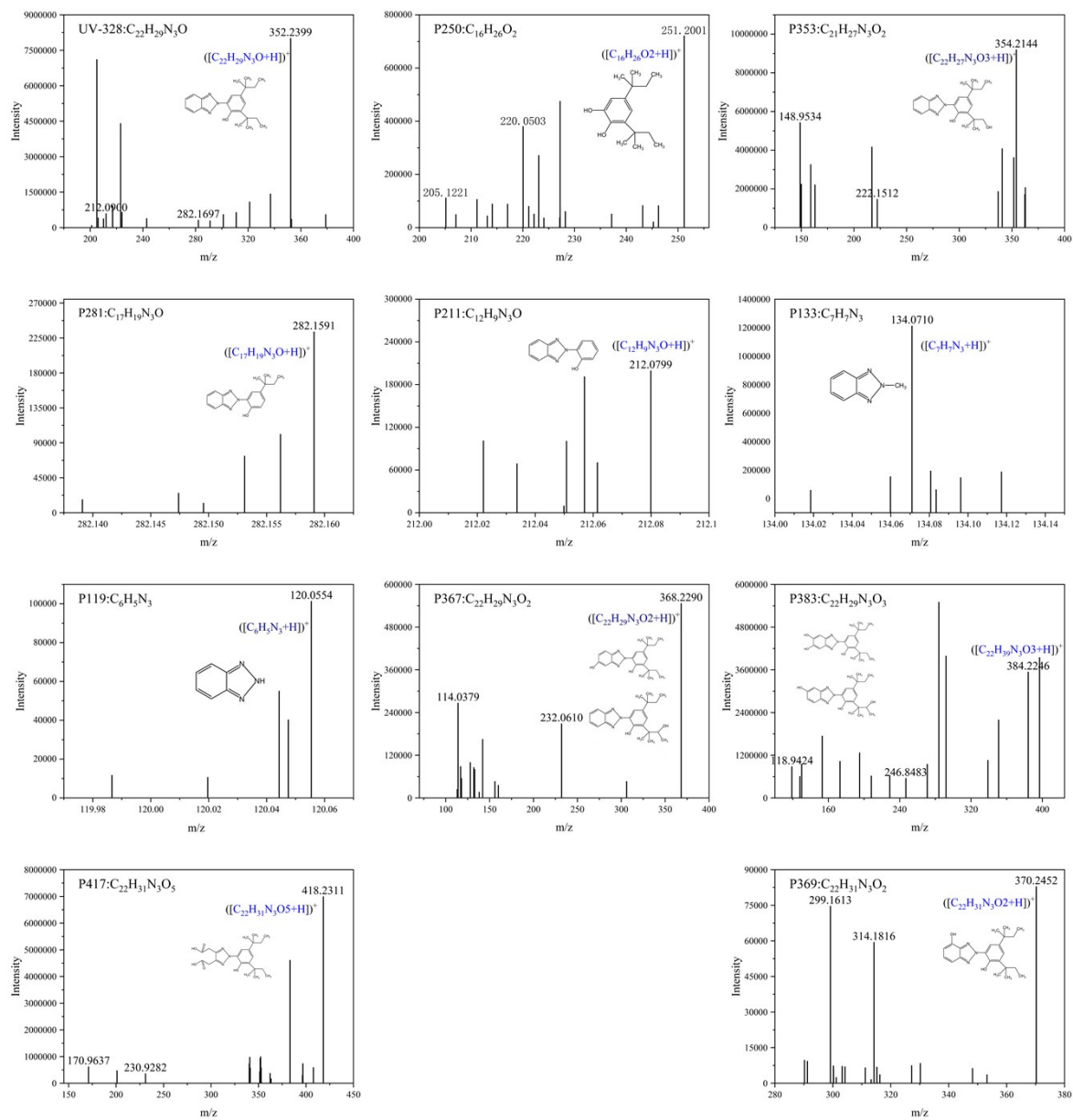


Fig. S9. Mass spectrum of photodegradation products.

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