Supplementary materials for:

Insights into the kinetics, theoretical model and mechanism of free radical synergistic degradation of micropollutants in UV/peroxydisulfate process

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different pH. Conditions: $[ACY]_0$ = 0.022 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, T = 20°C.

Figure S9 Determination of ATL by UV irradiation (a) and PDS oxidation (b) at different pH. Conditions: $[ATL]_0$ = 0.019 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, T = 20°C.

Figure S10 The apparent degradation rate constants of NB in direct UV photolysis and UV/PDS processes at different pHs. Conditions: $[NB]_0$ = 0.02 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, T = 20°C.

Figure S11 EPR spectra of $^{\bullet}OH$ and $SO_4^{\bullet-}$ adducts in UV/PDS process. Conditions: $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, pH = 6.0, T = 20°C.

Figure S12 Attenuation of PDS in UV/PDS process for the degradation of ACY (a) and ATL (b). Conditions: $[ACY]_0$ = 0.022 mM, $[ATL]_0$ = 0.019 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, pH = 6.0, T = 20°C.

Figure S13 Effect of SO_4^{2-} dosage on the k_{obs} of ACY (a) and ATL (b) degradation and specific rates of $^{\bullet}OH$ and $SO_4^{\bullet-}$ in the UV/PDS process. Conditions: $[ACY]_0$ = 0.022 mM, $[ATL]_0$ = 0.019 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, pH = 6.0 , T = 20°C.

Figure S14 Effect of NO_3^- dosage on the k_{obs} of ACY (a) and ATL (b) degradation and specific rates of $^{\bullet}OH$ and $SO_4^{\bullet-}$ in UV/PDS process. Conditions: $[ACY]_0$ = 0.022 mM, $[ATL]_0$ = 0.019mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, pH = 6.0 , T = 20°C.

Figure S15 Structural formula of ACY(a) and ATL(b).

Table S1. Principal reactions and rate constants in the UV/PDS system.

Table S2. Modeled steady-state concentrations of $^{\bullet}OH$ and $SO_4^{\bullet-}$ in different water matrices.

Table S3. Calculated condensed Fukui function and dual descriptor of ACY.[a]

Table S4. Calculated condensed Fukui function and dual descriptor of ATL.[a]

Table S5. Major intermediates of ACY detected in UV/PDS process.

Table S6. Major intermediates of ATL detected in UV/PDS process.

Text S1. Determination of $F_{p,o,UV}$ in the MVPS.

In a certain exposure time, only a part of water sample could receive the UV irradiation, while the remaining part was in the dark. Hence, by defining a reduction equivalent exposure time (t_{ree}, s) as the total reaction time (t, s) multiplied by the ratio of the exposure volume of the operation tube (πr^2 L, m^3) to the total sample volume (V, m^3), the UV ($F_{p,o,UV}$, einstein m^{-2}) photon fluence can be readily calculated as follows [1]:

$$t_{\text{ree}} = \frac{\pi r^2 h}{V} t \tag{S1}$$

$$F_{p,o,UV} = E_{p,o,UV} t_{\text{ree}} \tag{S2}$$

Where t is the reaction time (s), V is the volume of reaction solution (m^3), r and h are the radius and length of the UV tube (m), respectively. $E_{p,o,UV}$ was the UV photon fluence rate (PFR) in UV (einstein m^{-2} s^{-1}), respectively. Hence, the total exposure photon fluence ($F_{p,o}$, einstein m^{-2}) in the UV tube is equal to the sum of $F_{p,o,UV}$.

Uridine (0.01 mM) was used as the chemical actinometer to determine the $F_{p,o,UV}$ in the MVPS, respectively. The $F_{p,o,UV}$ (einstein m^{-2}) could be calculated as follows:

$$F_{p,o,UV} = \frac{\mathrm{k_u}}{\ln(10)\times 0.1\times \varepsilon_\lambda \times \Phi_\mathrm{u}} \times \mathrm{t} \tag{S3}$$

Where k_u (s^{-1}) is the time-based pseudo-first-order rate constant for UV photolysis of uridine, the ε_λ (M^{-1} cm^{-1}) and Φ_u are the molar absorption coefficient and quantum yield of uridine at an exposure wavelength (λ), respectively. The ε_{254} and Φ_u values were reported to be 8775 M^{-1} cm^{-1} and 0.020, respectively [2].

Text S2. UPLC-Q-TOF-MS method

The ACY and ATL degradation intermediates in UV/PDS process were identified on an Agilent 1290 UPLC system equipped with Waters Acquity UPLC BEH C18 column (2.1×100 mm, 1.7 μm). The column was maintained at 30°C and the injection volume was 2 μL. Milli-Q water containing 0.1% formic acid (v/v) (A) and acetonitrile (B) were used as the mobile phases at a flow rate of 0.2 mL/min. The gradient elution program (time in min, % mobile phase B) was set as follows: (0, 10), (2, 10), (5, 60), (8, 60), (12, 90), (15, 90), (16, 10), and (19, 10).

An Agilent 6545B MS Q-TOF, equipped with an electrospray ionization (ESI) source and operated in the positive ion mode, was employed to analyze degradation intermediates. The high-resolution mass spectra were collected from m/z 50 to 1500. The MS system was operated under the following conditions: capillary voltage 3.5 kV, drying gas temperature 320°C, drying gas flow rate 8 L/min, sheath gas temperature 350°C, sheath gas flow 11 L/min, nebulizing gas pressure 35 psi, and nozzle voltage 1.0 kV. The reference masses were 121.05087300 and 922.00979800 under ESI+ mode. The MassHunter Workstation Software (B.04.00, Agilent) was employed for both instrument control and data acquisition/analysis.

Text S3. Determination of the second-order reaction rate constants.

The parachlorobenzoic acid (pCBA) and benzoic acid (BA) were employed as the reference compounds in UV/H_2O_2 and UV/PDS processes due to their known reaction rate constants reacting with two radicals ($k_{\bullet OH,pCBA}$ =5×10^9 M^{-1} s^{-1} and $k_{SO_4^{\bullet -},BA}$ =1.2×10^9 M^{-1} s^{-1}) [3].

Because the reactions between ACY, ATL or pCBA and H_2O_2 are negligible, the function of ACY, ATL, and pCBA removal in UV/H_2O_2 process can be expressed as Eqs. (S4-S6):

$$-\frac{d[ACY]}{dt}=k_{UV,ACY}[ACY]+k_{^{\bullet}OH,ACY}[ACY] \tag{S4}$$

$$-\frac{d[ATL]}{dt}=k_{UV,ATL}[ATL]+k_{^{\bullet}OH,ATL}[ATL] \tag{S5}$$

$$-\frac{d[pCBA]}{dt}=k_{UV,pCBA}[pCBA]+k_{^{\bullet}OH,pCBA}[pCBA] \tag{S6}$$

Where $k_{UV,ACY}$, $k_{UV,ATL}$, and $k_{UV,pCBA}$ represent the direct UV photolysis rate constants (s^{-1}) of ACY, ATL, and pCBA, respectively. $k_{^{\bullet}OH,ACY}$ and $k_{^{\bullet}OH,ATL}$ can be calculated by Eqs. (S7) and (S8):

$$\frac{k_{^{\bullet}OH,ACY}[ACY]}{k_{^{\bullet}OH,pCBA}[pCBA]}=-\frac{\frac{d[ACY]}{dt}+k_{UV,ACY}[ACY]}{\frac{d[pCBA]}{dt}+k_{UV,pCBA}[pCBA]} \tag{S7}$$

$$\frac{k_{^{\bullet}OH,ATL}[ATL]}{k_{^{\bullet}OH,pCBA}[pCBA]}=-\frac{\frac{d[ATL]}{dt}+k_{UV,ATL}[ATL]}{\frac{d[pCBA]}{dt}+k_{UV,pCBA}[pCBA]} \tag{S8}$$

Similarly, the reaction between ACY, ATL, or BA and PDS are negligible as well. Hence, the function of ACY, ATL, and BA removal in UV/PDS process can be expressed as Eqs. (S9-S11).

$$-\frac{d[ACY]}{dt}=k_{UV,ACY}[ACY]+k_{SO_4^{\bullet-},ACY}[ACY] \tag{S9}$$

$$-\frac{d[ATL]}{dt}=k_{UV,ATL}[ATL]+k_{SO_4^{\bullet-},ATL}[ATL] \tag{S10}$$

$$-\frac{d[BA]}{dt}=k_{UV,BA}[BA]+k_{SO_4^{\bullet-},BA}[BA] \tag{S11}$$

where $k_{UV,BA}$ represents the direct UV photolysis rate constant (s^{-1}) of BA. Therefore, the $k_{SO_4^{\bullet-},ACY}$ and $k_{SO_4^{\bullet-},ATL}$ could be calculated by Eqs. (S12) and (S13).

$$\frac{k_{SO_4^{\bullet-},ACY}[ACY]}{k_{SO_4^{\bullet-},BA}[BA]} = -\frac{\frac{d[ACY]}{dt} + k_{UV,ACY}[ACY]}{\frac{d[BA]}{dt} + k_{UV,BA}[BA]} \tag{S12}$$

$$\frac{k_{SO_4^{\bullet-},ACY}[ATL]}{k_{SO_4^{\bullet-},BA}[BA]} = -\frac{\frac{d[ATL]}{dt} + k_{UV,ACY}[ATL]}{\frac{d[BA]}{dt} + k_{UV,BA}[BA]} \tag{S13}$$

Text S4. Calculation of condensed Fukui function.

Fukui function is an important conception in conceptual density functional theory, which has been widely used to predict the regioselectivity of electrophilic, nucleophilic, and radical attacks. Fukui function is defined as Eq (S14) [3].

$$f(r) = [\frac{\partial \mu}{\partial v(r)}]_N = [\frac{\partial \rho(\mathrm{r})}{\partial N}]_{v(r)} \tag{S14}$$

where $\rho(r)$ is the electron density at a point r in space, N is electron number in present system, the constant term v in the partial derivative is external potential. In the condensed version of Fukui function, atomic population number is used to represent the amount of electron density distribution around an atom. The condensed Fukui function (f) can be calculated as follows:[4]

Nucleophilic attack: $f_{\mathrm{A}}^{+} = q_{N}^{\mathrm{A}} - q_{N+1}^{\mathrm{A}}$ (S15)

Electrophilic attack: $f_{\mathrm{A}}^{-} = q_{N-1}^{\mathrm{A}} - q_{N}^{\mathrm{A}}$ (S16)

Radical attack: $f_{\mathrm{A}}^{0} = \left(q_{N-1}^{\mathrm{A}} - q_{N+1}^{\mathrm{A}}\right)/2$ (S17)

where q^{A} is the atomic charge of atom A at corresponding state. In this study, Hirshfeld charge was used to study reactive sites as it is considered to be one of the most suitable methods to calculate Fukui index.

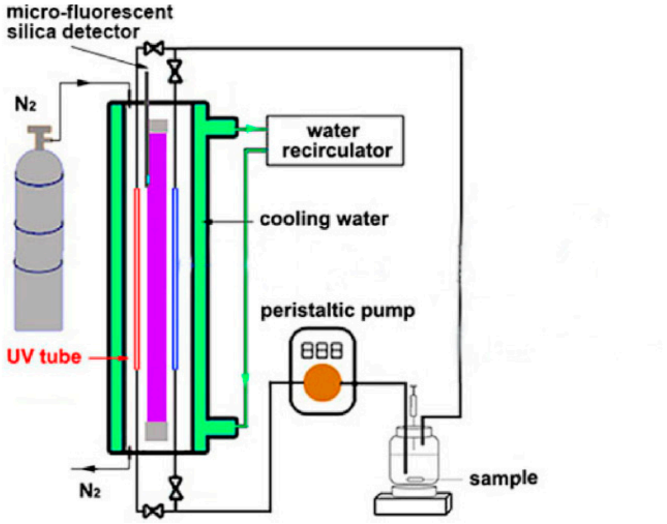

Figure S1. Schematic diagram of the MVPS [1].

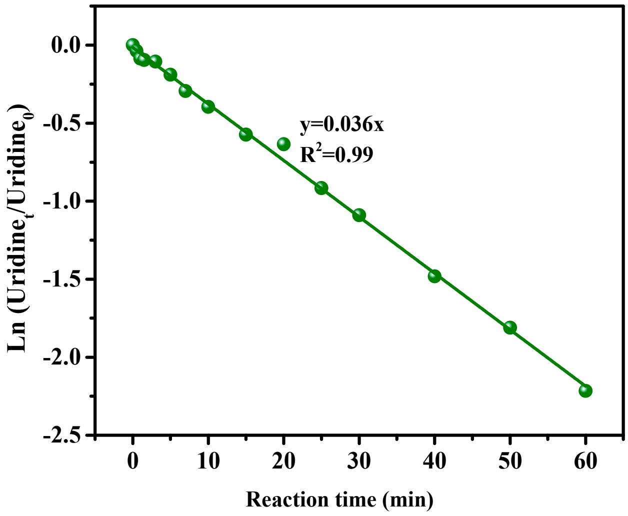

Figure S2 The degradation of uridine under direct UV photolysis. Conditions: [Uridine]$_0$ = 0.01 mM, pH=6.0, T = 20°C.

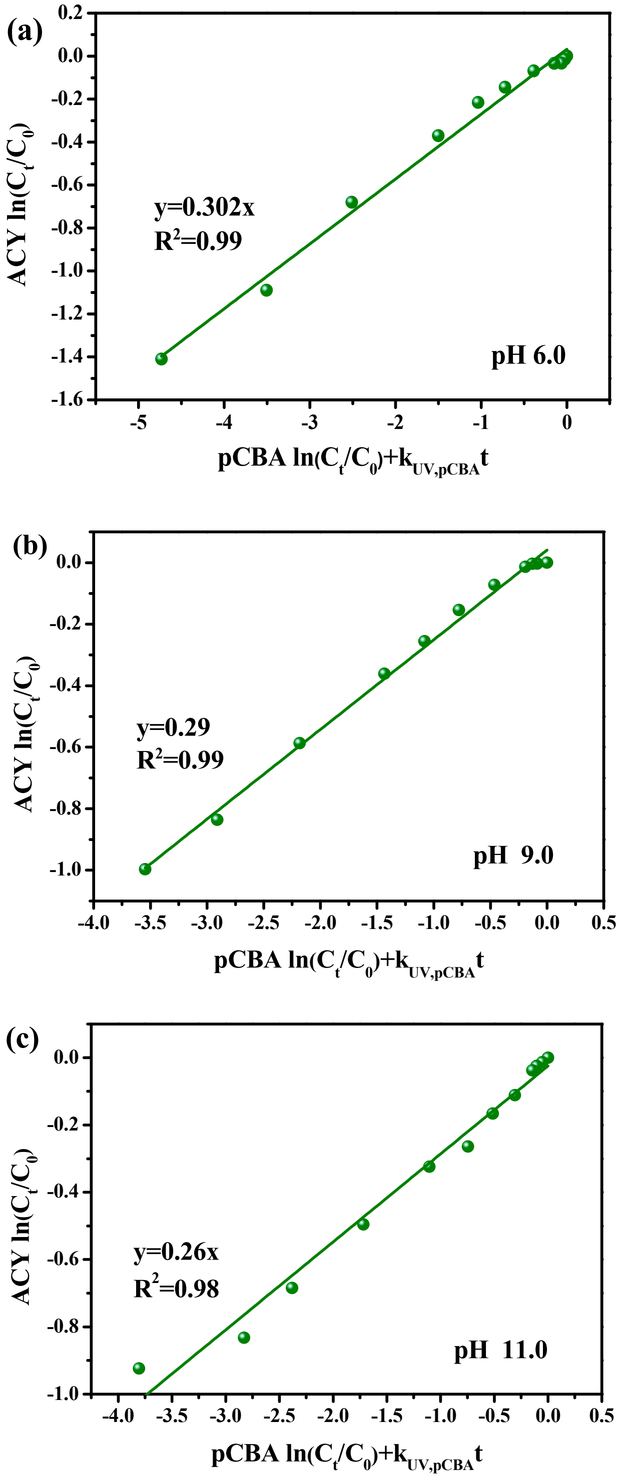

Figure S3 Determination of the second-order rate constant for the reaction of ACY with $^{\bullet}OH$ at pH=6.0 (a), pH=9.0 (b), and pH=11.0 (c). Conditions: $[ACY]_0$ = 0.022 mM, $[pCBA]_0$ = 0.022 mM, $[H_2O_2]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, T = 20°C.

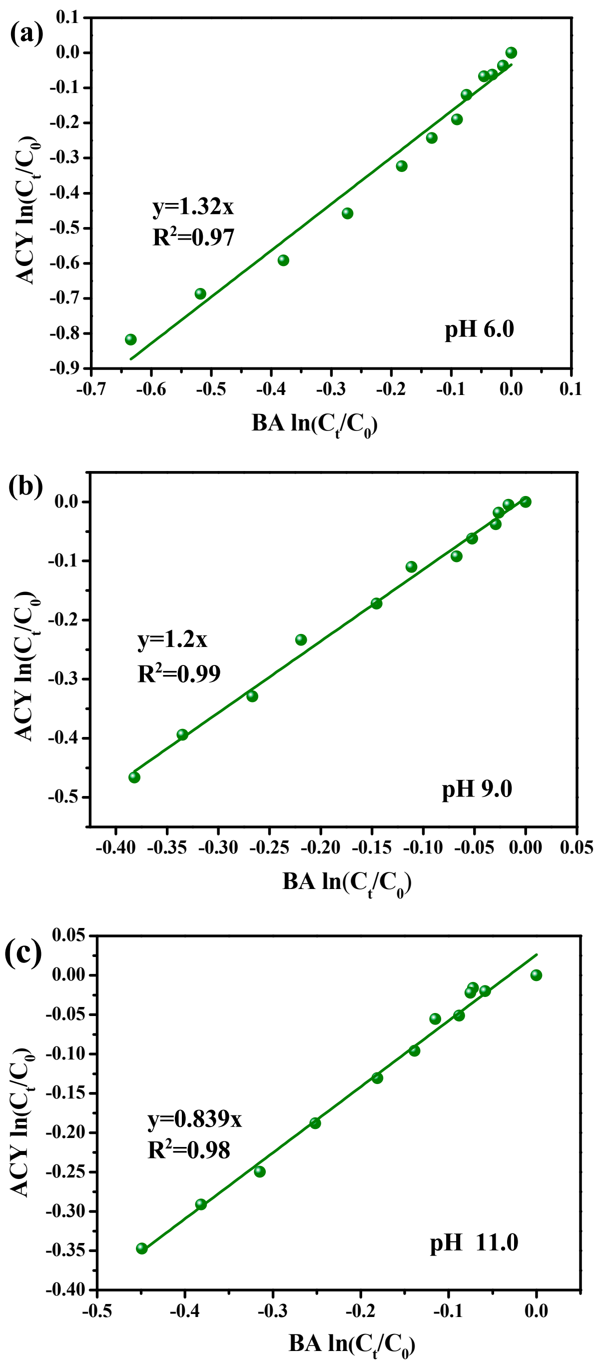

Figure S4 Determination of the second-order rate constant for the reaction of ACY with $SO_4^{\bullet-}$ at pH=6.0 (a), pH=9.0 (b), and pH=11.0 (c). Conditions: $[ACY]_0$ = 0.022 mM, $[BA]_0$ = 0.022 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV} = 1.12\times10^{-3}$ einstein m^{-2} s^{-1}, T = 20°C.

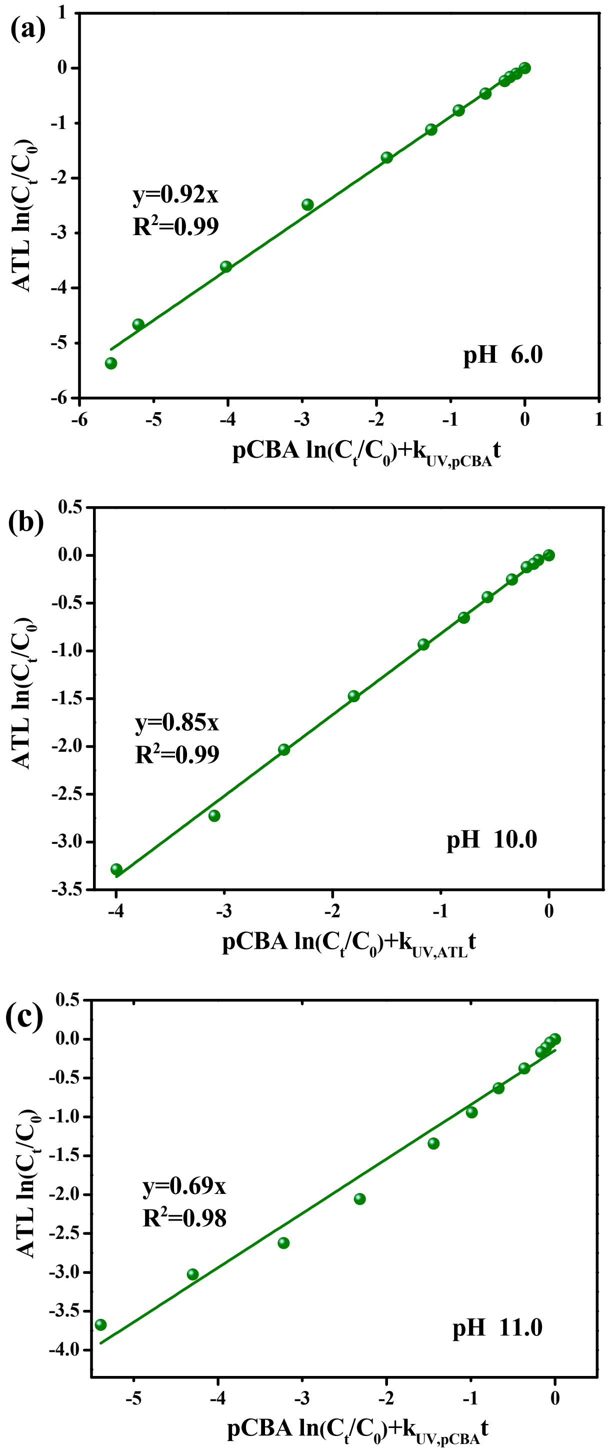

Figure S5 Determination of the second-order rate constant for the reaction of ATL with $^{\bullet}OH$ at pH=6.0 (a), pH=9.0 (b), and pH=11.0 (c). Conditions: $[ATL]_0$ = 0.019 mM, $[pCBA]_0$ = 0.019 mM, $[H_2O_2]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1} , T = 20°C.

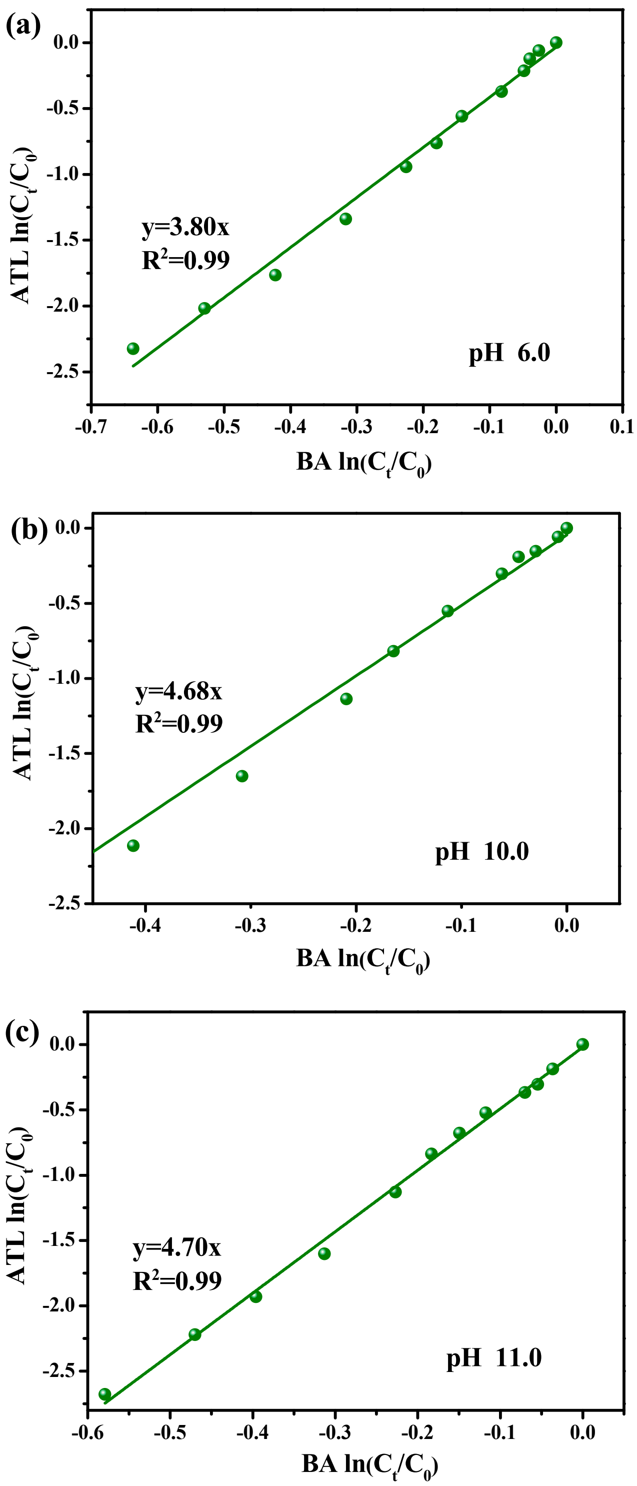

Figure S6 Determination of the second-order rate constant for the reaction of ATL with $SO_4^{\bullet-}$ pH=6.0 (a), pH=9.0 (b), and pH=11.0 (c). Conditions: $[ATL]_0$ = 0.019 mM, $[pCBA]_0$ = 0.019 mM, $[H_2O_2]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, T = 20°C.

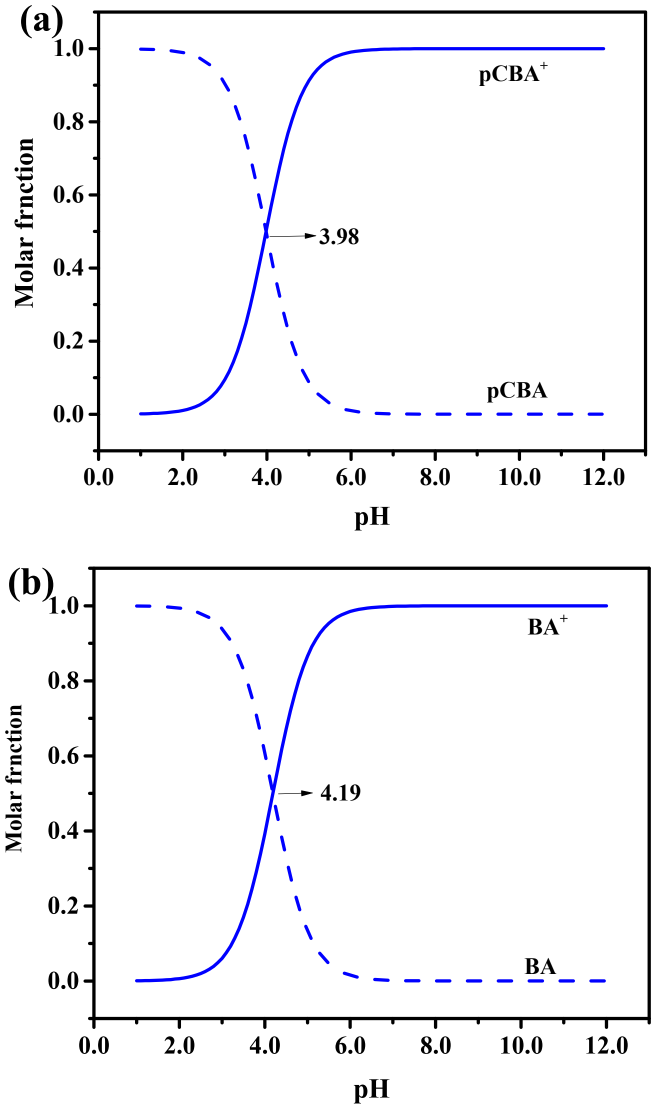

Figure S7 The existence forms of competing substrates pCBA(a) and BA(b) at different pH. Conditions: $[ATL]_0 = 0.019$ mM, $[PDS]_0 = 0.6$ mM, $E_{p,o,UV} = 1.12\times10^{-3}$ einstein m^{-2} s^{-1}, T = 20°C.

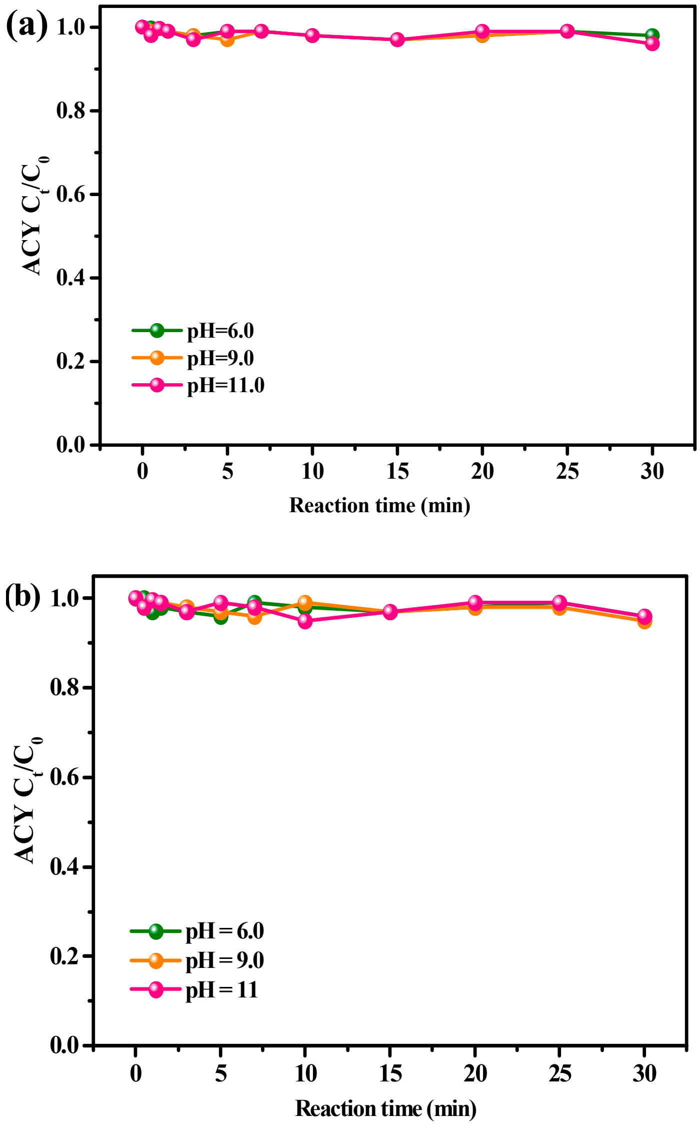

Figure S8 Determination of ACY by UV irradiation (a) and PDS oxidation (b) at different pH. Conditions: $[ACY]_0$ = 0.022 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV} = 1.12\times10^{-3}$ einstein m^{-2} s^{-1}, T = 20°C.

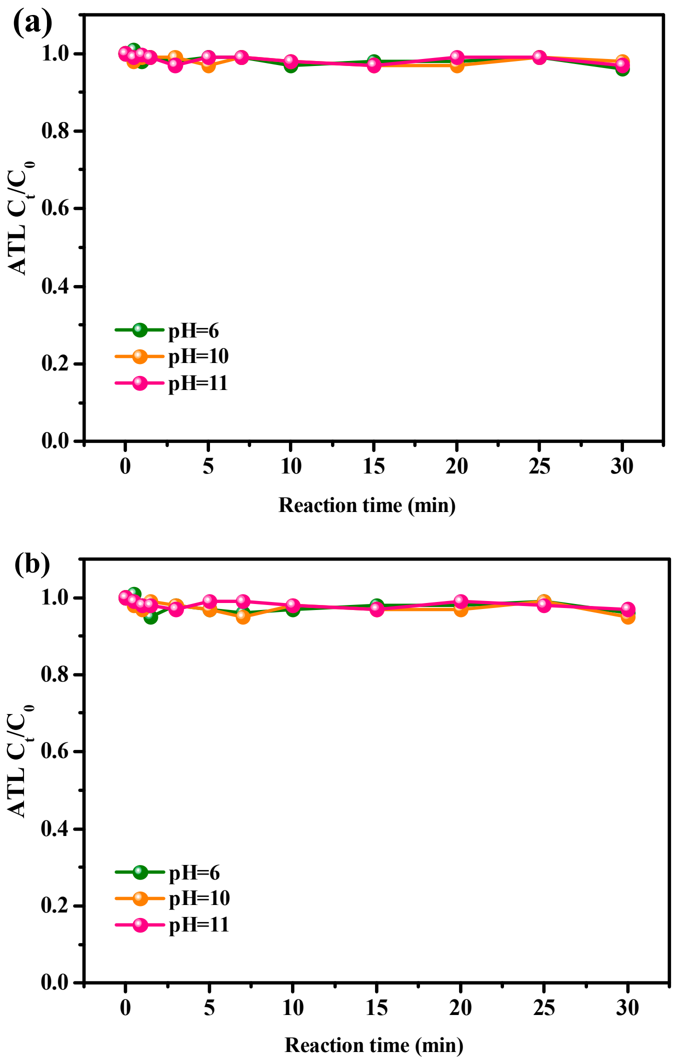

Figure S9 Determination of ATL by UV irradiation (a) and PDS oxidation (b) at different pH. Conditions: $[ATL]_0$ = 0.019 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV} = 1.12\times10^{-3}$ einstein m^{-2} s^{-1}, T = 20°C.

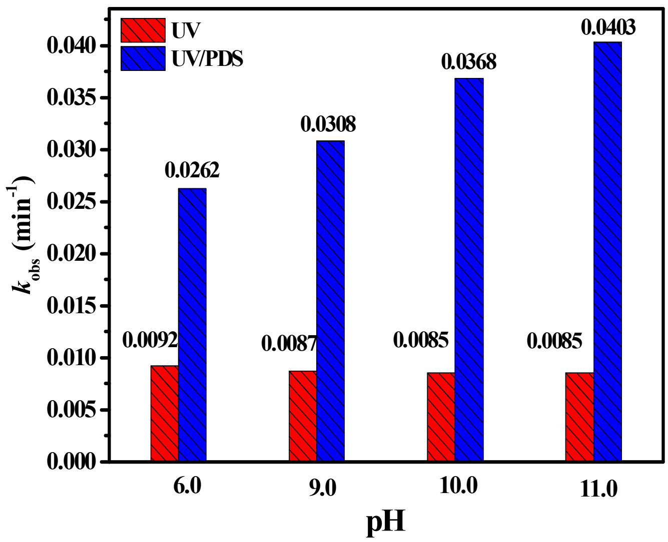

Figure S10 The apparent degradation rate constants of NB in direct UV photolysis and UV/PDS processes at different pHs. Conditions: $[NB]_0$ = 0.02 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, T = 20°C.

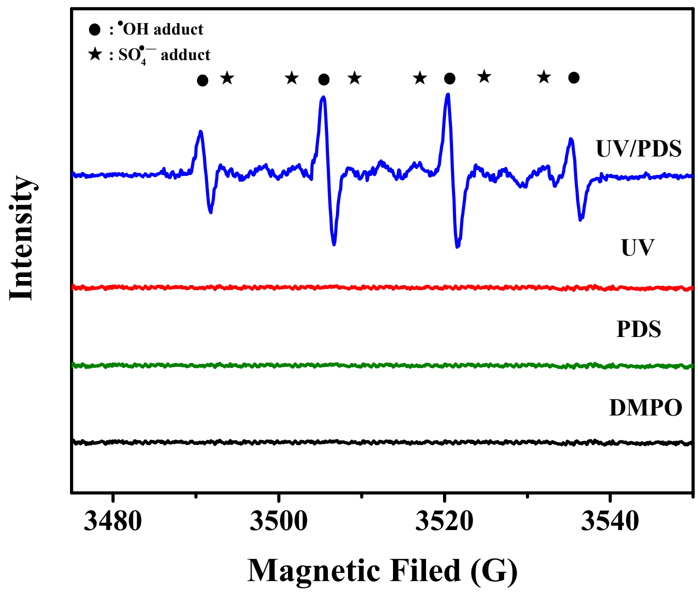

Figure S11 EPR spectra of $^{\bullet}$OH and $SO_4^{\bullet-}$ adducts in UV/PDS process. Conditions: $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, pH = 6.0, T = 20°C.

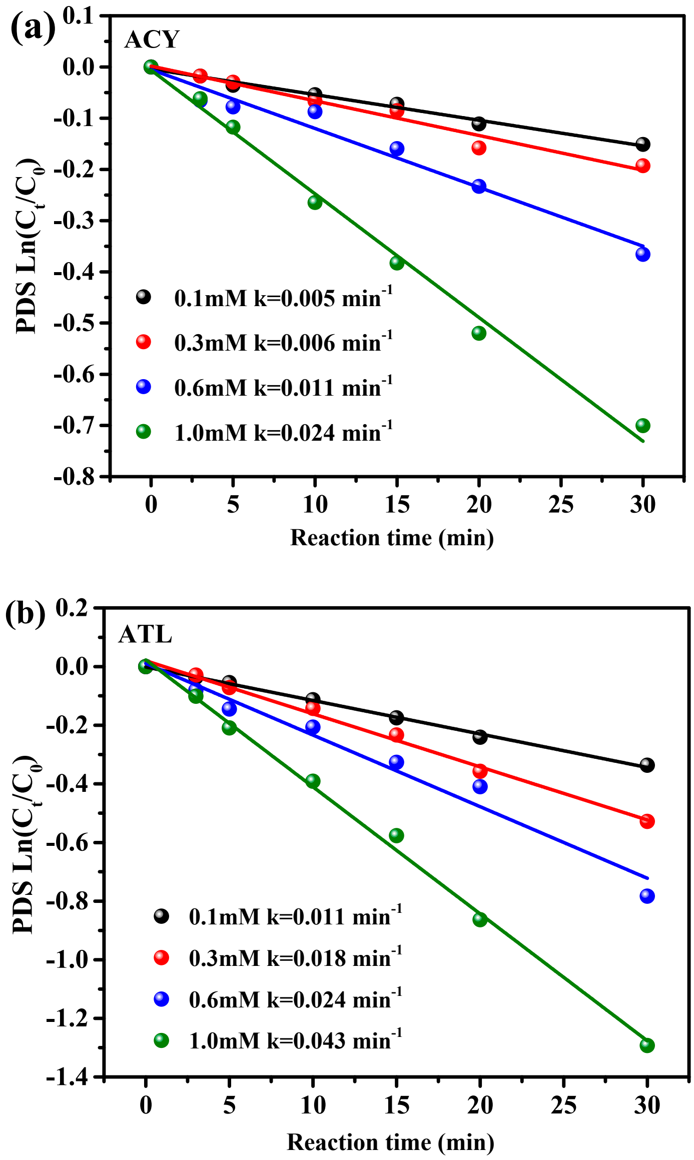

Figure S12 Attenuation of PDS in UV/PDS process for the degradation of ACY (a) and ATL (b). Conditions: $[ACY]_0$ = 0.022 mM, $[ATL]_0$ = 0.019 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV}$ = 1.12×10^{-3} einstein m^{-2} s^{-1}, pH = 6.0, T = 20°C.

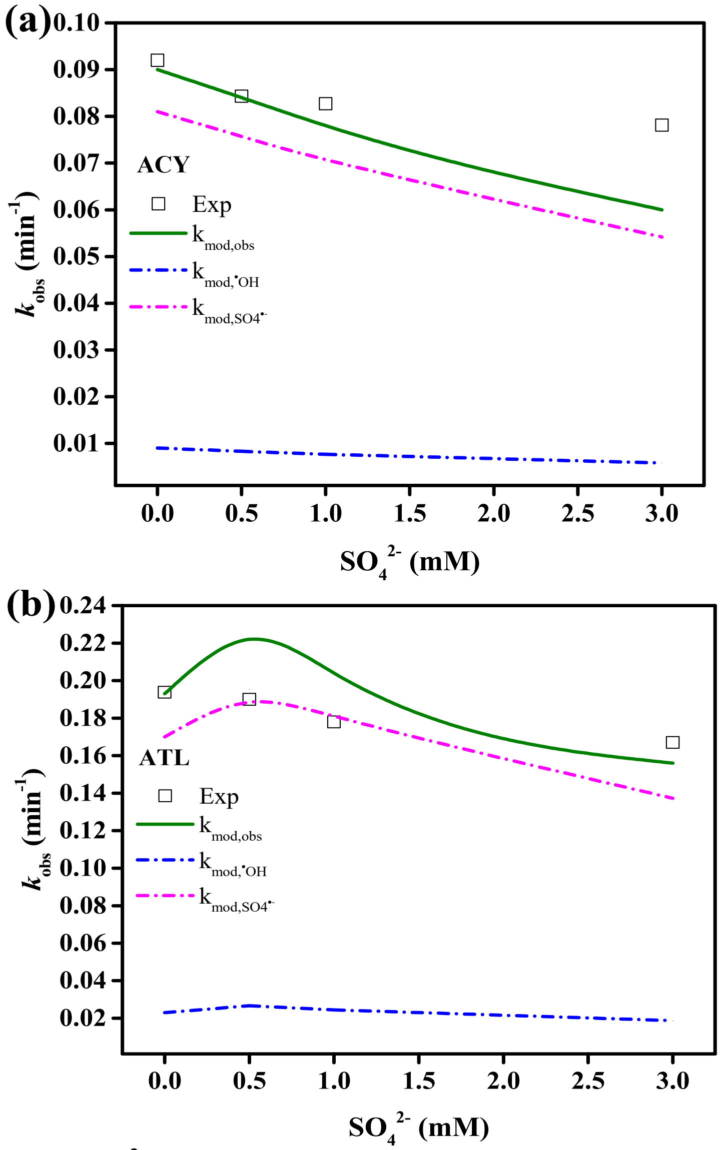

Figure S13 Effect of SO_4^{2-} dosage on the k_{obs} of ACY (a) and ATL (b) degradation and specific rates of $^{\bullet}OH$ and $SO_4^{\bullet-}$ in the UV/PDS process. Conditions: $[ACY]_0$ = 0.022 mM, $[ATL]_0$ = 0.019 mM, $[PDS]_0$ = 0.6 mM, $E_{p,o,UV} = 1.12\times10^{-3}$ einstein m^{-2} s^{-1}, pH = 6.0 , T = 20°C.

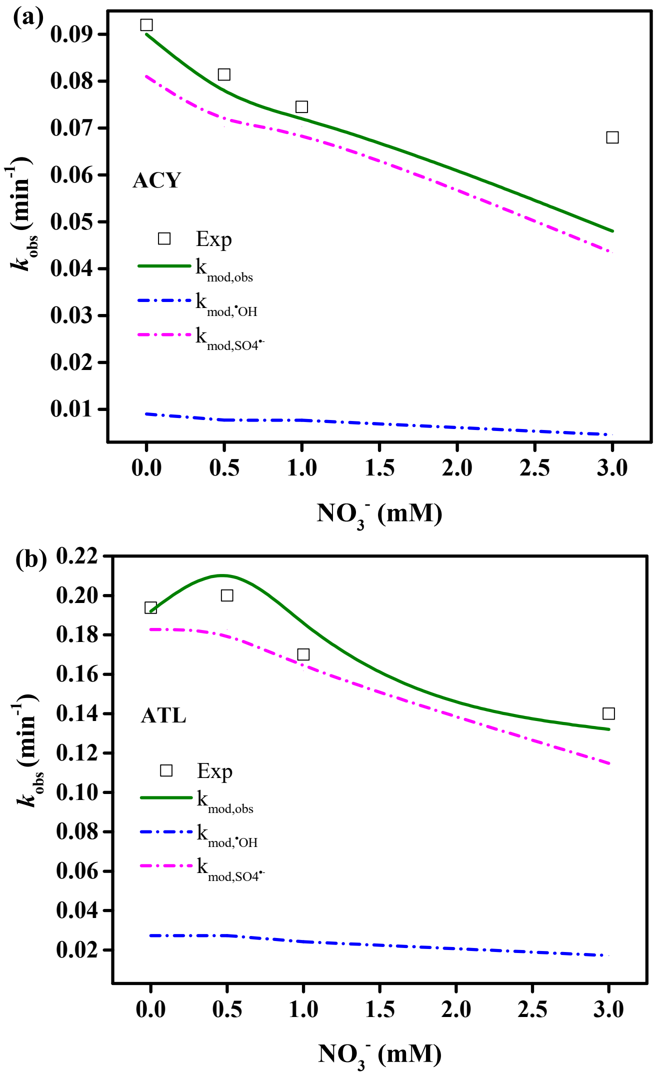

Figure S14 Effect of NO_3^- dosage on the k_{obs} of ACY (a) and ATL (b) degradation and specific rates of $^{\bullet}OH$ and $SO_4^{\bullet-}$ in UV/PDS process. Conditions: $[ACY]_0 = 0.022$ mM, $[ATL]_0 = 0.019$mM, $[PDS]_0 = 0.6$ mM, $E_{p,o,UV} = 1.12\times10^{-3}$ einstein m^{-2} s^{-1}, pH = 6.0 , T = 20°C.

(a)

(b)

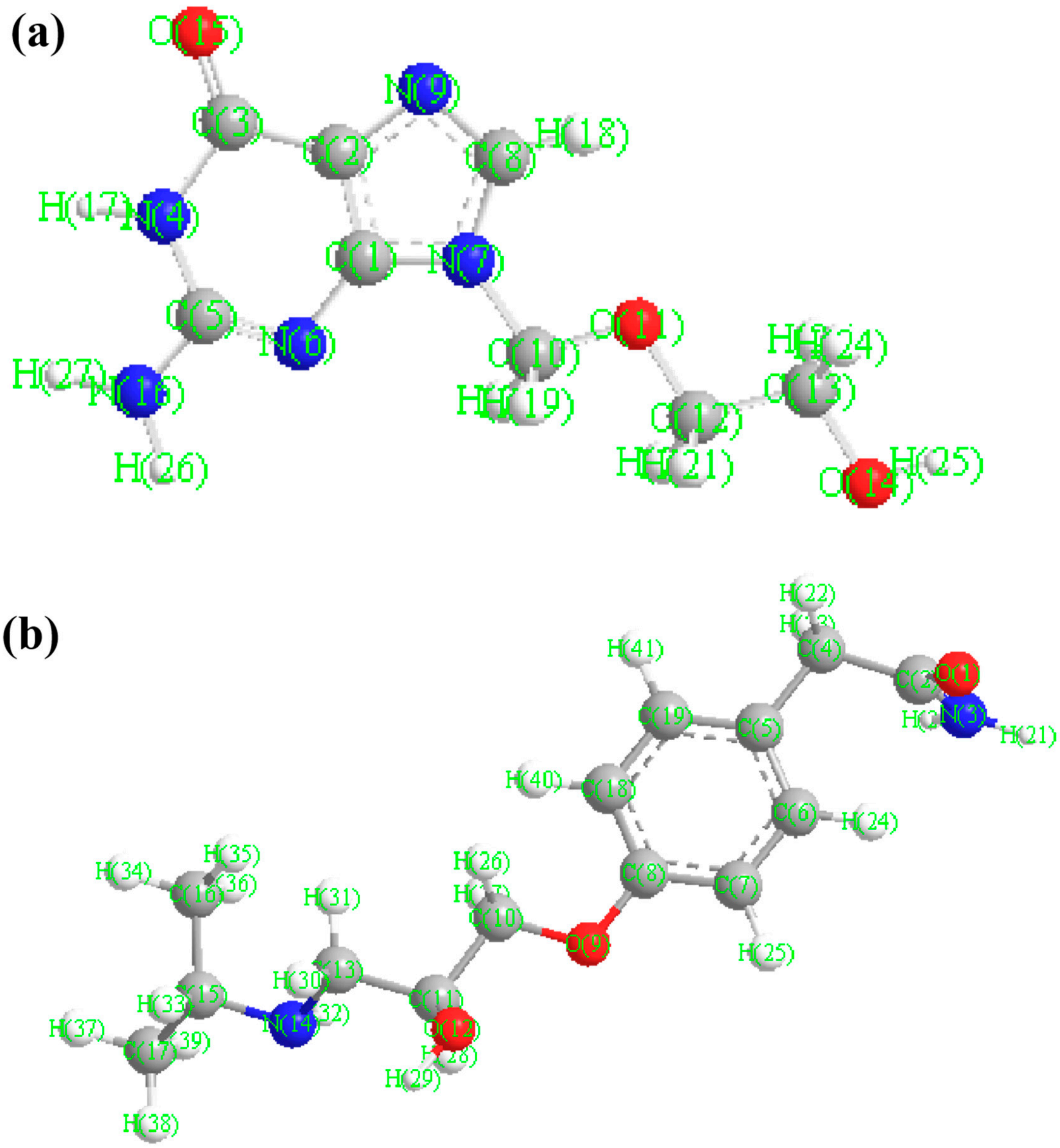

Figure S15 Structural formula of ACY(a) and ATL(b).

Table S1. Principal reactions and rate constants in the UV/PDS system.

No	Reaction	Rate Constant	Reference
Photolysis of PDS			
1	$S_2O_8^{2-} + hv \rightarrow 2SO_4^{\bullet-}$	$r_{SO_4^{\bullet-},form} = \Phi_{SO_4^{\bullet-}} I_0 f_{S_2O_8^{2-}} \left(1-10^{-Al}\right)$	[5]
$^{\bullet}OH$ and $SO_4^{\bullet-}$ reactions[6]			
2	$H_2O \rightarrow H^+ + OH^-$	1.0×10^3 s^{-1}	[6]
3	$H^+ + OH^- \rightarrow H_2O$	1.0×10^{11} M^{-1} s^{-1}	[6]
4	$H_2O_2 \rightarrow HO_2^- + H^+$	1.3×10^{-1} s^{-1}	[6]
5	$HO_2^- + H^+ \rightarrow H_2O_2$	5.0×10^{10} M^{-1} s^{-1}	[6]
6	$HO_2^{\bullet} \rightarrow O_2^{\bullet-} + H^+$	7.0×10^5 s^{-1}	[7]
7	$O_2^{\bullet-} + H^+ \rightarrow HO_2^{\bullet}$	5.0×10^{10} M^{-1} s^{-1}	[7]
8	$HO_2^{\bullet} + O_2^{\bullet-} \rightarrow HO_2^- + O_2$	9.7×10^7 M^{-1} s^{-1}	[7]
9	$HO_2^{\bullet} + HO_2^{\bullet} \rightarrow H_2O_2 + O_2$	8.3×10^5 M^{-1} s^{-1}	[6]

No	Reaction	Rate Constant	Reference
10	$^{\bullet}OH + ^{\bullet}OH \rightarrow H_2O_2$	5.5×10^{9} M^{-1} s^{-1}	[6]
11	$^{\bullet}OH + HO_2^{\bullet} \rightarrow H_2O + O_2$	7.1×10^{9} M^{-1} s^{-1}	[7]
12	$^{\bullet}OH + O_2^{\bullet-} \rightarrow OH^{-} + O_2$	1.0×10^{10} M^{-1} s^{-1}	[7]
13	$^{\bullet}OH + H_2O_2 \rightarrow HO_2^{\bullet} + H_2O$	2.7×10^{7} M^{-1} s^{-1}	[8]
14	$^{\bullet}OH + HO_2^{-} \rightarrow H_2O + O_2^{\bullet-}$	7.5×10^{9} M^{-1} s^{-1}	[8]
15	$2H_2O_2 \rightarrow 2H_2O + O_2$	2.3×10^{-2} s^{-1}	[6]
16	$SO_4^{\bullet-} + SO_4^{\bullet-} \rightarrow S_2O_8^{2-}$	4.0×10^{8} M^{-1} s^{-1}	[8]
17	$SO_4^{\bullet-} + OH^{-} \rightarrow ^{\bullet}OH + SO_4^{2-}$	6.5×10^{7} M^{-1} s^{-1}	[8]
18	$^{\bullet}OH + SO_4^{\bullet-} \rightarrow HSO_5^{-}$	1.0×10^{10} M^{-1} s^{-1}	[8]
19	$^{\bullet}OH + HSO_5^{-} \rightarrow SO_5^{\bullet-} + H_2O$	1.7×10^{7} M^{-1} s^{-1}	[8]
20	$SO_4^{\bullet-} + HSO_5^{-} \rightarrow SO_5^{\bullet-} + HSO_4^{-}$	1.0×10^{5} M^{-1} s^{-1}	[9]
21	$SO_4^{\bullet-} + S_2O_8^{2-} \rightarrow SO_4^{2-} + S_2O_8^{\bullet-}$	6.1×10^{5} M^{-1} s^{-1}	[9]

No	Reaction	Rate Constant	Reference
22	$SO_4^{\bullet-} + H_2O \rightarrow HSO_4^- + {}^{\bullet}OH$	5.0×10^2 M^{-1} s^{-1}	[8]
23	$HSO_4^- + {}^{\bullet}OH \rightarrow SO_4^{\bullet-} + H_2O$	6.9×10^5 M^{-1} s^{-1}	[8]
24	$2SO_5^{\bullet-} \rightarrow 2SO_4^{\bullet-} + O_2$	1.0×10^8 s^{-1}	[8]
25	$HSO_4^- \rightarrow SO_4^{2-} + H^+$	1.2×10^{-2} s^{-1}	[8]
In the presence of HCO_3^-			
26	$SO_4^{\bullet-}+HCO_3^-\rightarrow CO_3^{\bullet-}+SO_4^{2-} + H^+$	9.1×10^6 M^{-1} s^{-1}	[10]
27	$SO_4^{\bullet-} + CO_3^{2-} \rightarrow CO_3^{\bullet-} + SO_4^{2-}$	4.1×10^6 M^{-1} s^{-1}	[10]
28	${}^{\bullet}OH + HCO_3^- \rightarrow CO_3^{\bullet-}+ H_2O$	8.5×10^6 M^{-1} s^{-1}	[10]
29	${}^{\bullet}OH + CO_3^{2-} \rightarrow CO_3^{\bullet-} + OH^-$	3.9×10^8 M^{-1} s^{-1}	[10]
30	${}^{\bullet}OH + H_2CO_3 \rightarrow CO_3^{\bullet-} + H_2O + H^+$	1.0×10^6 M^{-1} s^{-1}	[10]
31	${}^{\bullet}OH + CO_3^{\bullet-} \rightarrow$ products	3.0×10^9 M^{-1} s^{-1}	[10]
32	$CO_3^{\bullet-}+ CO_3^{\bullet-} \rightarrow$ products	3.0×10^7 M^{-1} s^{-1}	[10]

No	Reaction	Rate Constant	Reference
33	$HCO_3^- + H^+ \rightarrow H_2CO_3$	1.0×10^{10} M^{-1} s^{-1}	[10]
34	$H_2CO_3 \rightarrow HCO_3^- + H^+$	5.0×10^5 s^{-1}	[10]
35	$CO_3^{2-} + H^+ \rightarrow HCO_3^-$	5.0×10^{10} M^{-1} s^{-1}	[10]
36	$HCO_3^- \rightarrow CO_3^{2-} + H^+$	2.5 s^{-1}	[10]
In the presence of Cl^-			
37	$HCl \rightarrow H^+ + Cl^-$	8.6×10^{16} s^{-1}	[6]
38	$H^+ + Cl^- \rightarrow HCl$	5.0×10^{10} M^{-1} s^{-1}	[6]
39	$HClO \rightarrow H^+ + ClO^-$	1.6×10^3 s^{-1}	[6]
40	$H^+ + ClO^- \rightarrow HClO$	5.0×10^{10} M^{-1} s^{-1}	[6]
41	$Cl^- + {}^{\bullet}OH \rightarrow ClOH^{\bullet-}$	4.3×10^9 M^{-1} s^{-1}	[6]
42	$ClOH^{\bullet-} + Cl^- \rightarrow Cl_2^{\bullet-} + OH^-$	1.0×10^5 M^{-1} s^{-1}	[6]
43	$ClOH^{\bullet-} \rightarrow Cl^- + {}^{\bullet}OH$	6.1×10^9 s^{-1}	[6]

No	Reaction	Rate Constant	Reference
44	$ClOH^{\bullet-} + H^+ \rightarrow Cl^\bullet + H_2$	2.1×10^{10} M^{-1} s^{-1}	[6]
45	$Cl^- + Cl^\bullet \rightarrow Cl_2^{\bullet-}$	6.5×10^9 M^{-1} s^{-1}	[6]
46	$Cl^- + Cl_2 \rightarrow Cl_3^-$	2.0×10^4 M^{-1} s^{-1}	[6]
47	$Cl^- + HClO \rightarrow Cl_2OH^-$	1.5×10^4 M^{-1} s^{-1}	[7]
48	$Cl^\bullet + H_2O_2 \rightarrow HCl + HO_2^\bullet$	4.0×10^9 M^{-1} s^{-1}	[7]
49	$Cl^\bullet + OH^- \rightarrow ClOH^{\bullet-}$	1.8×10^{10} M^{-1} s^{-1}	[6]
50	$Cl^\bullet + Cl^\bullet \rightarrow Cl_2$	1.0×10^8 M^{-1} s^{-1}	[6]
51	$Cl^\bullet + H_2O \rightarrow HClOH$	2.5×10^5 M^{-1} s^{-1}	[6]
52	$Cl^\bullet + H_2O \rightarrow ClOH^{\bullet-} + H^+$	1.6×10^5 M^{-1} s^{-1}	[6]
53	$Cl_2^{\bullet-} + O_2^{\bullet-} \rightarrow 2Cl^- + O_2$	1.0×10^9 M^{-1} s^{-1}	[6]
54	$Cl_2^{\bullet-} + OH^- \rightarrow ClOH^{\bullet-} + Cl^-$	4.5×10^7 M^{-1} s^{-1}	[6]
55	$Cl_2^{\bullet-} \rightarrow Cl^\bullet + Cl^-$	1.1×10^5 s^{-1}	[6]

No	Reaction	Rate Constant	Reference
56	$Cl_2^{\bullet-} + Cl_2^{\bullet-} \rightarrow Cl_2 + 2Cl^-$	8.3×10^8 M^{-1} s^{-1}	[6]
57	$Cl_2^{\bullet-} + H_2O_2 \rightarrow 2Cl^- + HO_2^\bullet + H^+$	1.4×10^5 M^{-1} s^{-1}	[6]
58	$Cl_2^{\bullet-} + H_2O \rightarrow HClOH + Cl^-$	1.3×10^3 M^{-1} s^{-1}	[6]
59	$Cl_2^{\bullet-} + {}^\bullet OH \rightarrow HClO + Cl^-$	1.0×10^9 M^{-1} s^{-1}	[6]
60	$HClOH \rightarrow ClOH^{\bullet-} + H^+$	1.0×10^8 M^{-1} s^{-1}	[6]
61	$HClOH \rightarrow Cl^\bullet + H_2O$	1.0×10^2 s^{-1}	[6]
62	$HClOH + Cl^- \rightarrow Cl_2^{\bullet-} + H_2O$	5.0×10^9 M^{-1} s^{-1}	[6]
63	$Cl_3^- + HO_2^\bullet \rightarrow Cl_2^{\bullet-} + HCl + O_2$	1.0×10^9 M^{-1} s^{-1}	[6]
64	$Cl_3^- + O_2^{\bullet-} \rightarrow Cl_2^{\bullet-} + Cl^- + O_2$	3.8×10^9 M^{-1} s^{-1}	[6]
65	$Cl_3^- \rightarrow Cl_2 + Cl^-$	1.1×10^5 s^{-1}	[6]
66	$Cl_2 + O_2^{\bullet-} \rightarrow Cl_2^{\bullet-} + O_2$	1.0×10^9 M^{-1} s^{-1}	[6]
67	$Cl_2 + HO_2^\bullet \rightarrow Cl_2^{\bullet-} + H^+ + O_2$	1.0×10^9 M^{-1} s^{-1}	[8]

No	Reaction	Rate Constant	Reference
68	$Cl_2 + H_2O \rightarrow Cl_2OH^- + H^+$	1.5×10^1 M^{-1} s^{-1}	[6]
69	$Cl_2 + H_2O_2 \rightarrow 2HCl + O_2$	1.3×10^4 M^{-1} s^{-1}	[6]
70	$Cl_2OH^- + H^+ \rightarrow Cl_2 + H_2O$	2.0×10^{10} M^{-1} s^{-1}	[6]
71	$Cl_2OH^- \rightarrow HClO + Cl^-$	5.5×10^9 s^{-1}	[6]
72	$HClO + {}^{\bullet}OH \rightarrow ClO^{\bullet} + H_2O$	2.0×10^9 M^{-1} s^{-1}	[8]
73	$HClO + O_2^{\bullet-} \rightarrow Cl^{\bullet} + OH^- + O_2$	7.5×10^6 M^{-1} s^{-1}	[8]
74	$HClO + HO_2^{\bullet} \rightarrow Cl^{\bullet} + H_2O + O_2$	7.5×10^6 M^{-1} s^{-1}	[6]
75	$HClO + H_2O_2 \rightarrow HCl + H_2O + O_2$	1.1×10^4 M^{-1} s^{-1}	[6]
76	$ClO^- + {}^{\bullet}OH \rightarrow ClO^{\bullet} + OH^-$	8.8×10^9 M^{-1} s^{-1}	[6]
77	$ClO^- + H_2O_2 \rightarrow Cl^- + H_2O + O_2$	1.7×10^5 M^{-1} s^{-1}	[6]
78	$ClO^-+O_2^{\bullet-}+H_2O\rightarrow Cl^{\bullet}+ 2OH^- + O_2$	2.0×10^8 M^{-1} s^{-1}	[6]
79	$Cl_2^{\bullet-} + HO_2^{\bullet} \rightarrow 2Cl^- + H^+ + O_2$	3.0×10^9 M^{-1} s^{-1}	[6]

No	Reaction	Rate Constant	Reference
80	$Cl_2 + H_2O \rightarrow Cl_2OH^- + H^+$	1.5×10^1 M^{-1} s^{-1}	[6]
81	$SO_4^{\bullet-} + Cl^- \rightarrow SO_4^{2-} + Cl^\bullet$	4.7×10^8 M^{-1} s^{-1}	[9]
82	$SO_4^{2-} + Cl^\bullet \rightarrow SO_4^{\bullet-} + Cl^-$	2.5×10^8 M^{-1} s^{-1}	[9]
83	$OCl^- + CO_3^{\bullet-} \rightarrow CO_3^{2-} + ClO^\bullet$	5.7×10^5 M^{-1} s^{-1}	[11]
84	$Cl^\bullet + CO_3^{2-} \rightarrow CO_3^{\bullet-} + Cl^-$	5.0×10^8 M^{-1} s^{-1}	[11]
85	$Cl^\bullet + HCO_3^- \rightarrow CO_3^{\bullet-} + Cl^- + H^+$	2.2×10^8 M^{-1} s^{-1}	[11]
86	$Cl_2^{\bullet-} + CO_3^{2-} \rightarrow CO_3^{\bullet-} + 2Cl^-$	1.6×10^8 M^{-1} s^{-1}	[11]
87	$Cl_2^{\bullet-} + HCO_3^- \rightarrow CO_3^{\bullet-} + 2Cl^- + H^+$	8.0×10^7 M^{-1} s^{-1}	[11]
In the presence of NO_3^-			
88	$NO_3^\bullet + NO_3^\bullet \rightarrow N_2O_6$	7.9×10^5 M^{-1} s^{-1}	[11]
89	$NO_3^\bullet + Cl^- \rightarrow NO_3^- + Cl^\bullet$	7.1×10^7 M^{-1} s^{-1}	[11]
In the presence of NOM			

No	Reaction	Rate Constant	Reference
90	$SO_4^{\bullet-} + NOM \rightarrow$ products	$2.35 \times 10^7\ M^{-1}s^{-1}$	[10]
91	$HO^{\bullet} + NOM \rightarrow$ products	$3.0 \times 10^8\ M^{-1}\ s^{-1}$	[10]
92	$CO_3^{\bullet-} + NOM \rightarrow$ products	$2.8 \times 10^2\ M^{-1}\ s^{-1}$	[10]
93	$Cl^{\bullet} + NOM \rightarrow$ products	$1.3 \times 10^4\ M^{-1}\ s^{-1}$	[10]
In the presence of $HPO_4^{2-}/H_2PO_4^{-}$			
94	$SO_4^{\bullet-} + H_2PO_4^{-} \rightarrow$ products	$7.2 \times 10^4\ M^{-1}\ s^{-1}$	[10]
95	$SO_4^{\bullet-} + HPO_4^{2-} \rightarrow SO_4^{2-} + HPO_4^{\bullet-}$	$1.2 \times 10^6\ M^{-1}\ s^{-1}$	[10]
96	$^{\bullet}OH + H_2PO_4^{-} \rightarrow HPO_4^{\bullet-} + H_2O$	$1.5 \times 10^5\ M^{-1}\ s^{-1}$	[10]
97	$^{\bullet}OH + HPO_4^{2-} \rightarrow HPO_4^{\bullet-} + OH^{-}$	$2 \times 10^4\ M^{-1}\ s^{-1}$	[10]
98	$H_2PO_4^{-} + H^{+} \rightarrow H_3PO_4$	$5.0\times10^{10}\ M^{-1}\ s^{-1}$	[11]
99	$H_3PO_4 \rightarrow H^{+} + H_2PO_4^{-}$	$3.97\times10^8\ M^{-1}\ s^{-1}$	[11]
In the presence of Br^{-}			

No	Reaction	Rate Constant	Reference
100	$SO_4^{\bullet-} + Br^- \rightarrow SO_4^{2-} + Br^\bullet$	$3.5\times10^9\ M^{-1}\ s^{-1}$	[12]
101	$^\bullet OH + Br^- \rightarrow BrOH^{\bullet-}$	$1.1\times10^{10}\ M^{-1}\ s^{-1}$	[13]
102	$Br^\bullet + H_2O \rightarrow BrOH^{\bullet-} + H^+$	$1.4\ M^{-1}\ s^{-1}$	[13]
103	$Br^\bullet + OH^- \rightarrow BrOH^{\bullet-}$	$1.06\times10^{10}\ M^{-1}s^{-1}$	[14]
104	$BrOH^{\bullet-} \rightarrow {}^\bullet OH + Br^-$	$3.3\times10^7\ s^{-1}$	[14]
105	$BrOH^{\bullet-} \rightarrow Br^\bullet + OH^-$	$4.2\times10^6\ s^{-1}$	[14]
106	$BrOH^{\bullet-} + H^+ \rightarrow Br^\bullet + H_2O$	$4.4\times10^{10}\ M^{-1}\ s^{-1}$	[14]
107	$BrOH^{\bullet-} + Br^- \rightarrow Br_2^{\bullet-} + OH^-$	$1.9\times10^8\ M^{-1}\ s^{-1}$	[14]
108	$Br^\bullet + Br^- \rightarrow Br_2^{\bullet-}$	$1.2\times10^{10}\ M^{-1}\ s^{-1}$	[15]
109	$Br^\bullet + Br^\bullet \rightarrow Br_2$	$1.0\times10^9\ M^{-1}\ s^{-1}$	[13]
110	$Br^\bullet + H_2O_2 \rightarrow HO_2^\bullet + Br^- + H^+$	$4.0\times10^9\ M^{-1}\ s^{-1}$	[16]
111	$Br^\bullet + HO_2^\bullet \rightarrow Br^- + H^+ + O_2$	$1.6\times10^8\ M^{-1}\ s^{-1}$	[16]

No	Reaction	Rate Constant	Reference
112	$Br^{\bullet} + BrO^{-} \rightarrow BrO^{\bullet} + Br^{-}$	4.0×10^{9} M^{-1} s^{-1}	[17]
113	$Br_2^{\bullet-} \rightarrow Br^{\bullet} + Br^{-}$	1.9×10^{4} s^{-1}	[15]
114	$Br_2^{\bullet-} + Br_2^{\bullet-} \rightarrow Br_2 + 2Br^{--}$	1.9×10^{9} M^{-1} s^{-1}	[18]
115	$Br_2^{\bullet-} + Br^{\bullet} \rightarrow Br_2 + Br^{-}$	2.0×10^{9} M^{-1} s^{-1}	[17]
116	$Br_2^{\bullet-} + H_2O_2 \rightarrow HO_2^{\bullet} + 2Br^{-} + H^{+}$	5.0×10^{2} M^{-1} s^{-1}	[19]
117	$Br_2^{\bullet-} + HO_2^{\bullet} \rightarrow HBr + Br + O_2$	1.0×10^{8} M^{-1} s^{-1}	[17]
118	$Br_2^{\bullet-} + HO_2^{\bullet} \rightarrow Br_2 + HO_2^{-}$	4.4×10^{9} M^{-1} s^{-1}	[18]
119	$Br_2^{\bullet-} + O_2^{\bullet-} \rightarrow Br^{-} + Br^{-} + O_2$	1.7×10^{8} M^{-1} s^{-1}	[16]
120	$Br_2^{\bullet-} + BrO^{-} \rightarrow BrO^{\bullet} + 2Br^{-}$	6.2×10^{7} M^{-1} s^{-1}	[17]
121	$Br_2^{\bullet-} + HO^{\bullet} \rightarrow HOBr + Br^{-}$	1.0×10^{9} M^{-1} s^{-1}	[16]
122	$Br_2^{\bullet-} + OH^{-} \rightarrow BrOH^{\bullet-} + Br^{-}$	2.7×10^{6} M^{-1} s^{-1}	[19]
123	$Br_2 + Br^{-} \rightarrow Br_3^{-}$	9.6×10^{8} M^{-1} s^{-1}	[15]

No	Reaction	Rate Constant	Reference
124	$Br_2 + HO_2^{\bullet} \rightarrow Br_2^{\bullet-} + O_2 + H^+$	$1.1\times10^8\ M^{-1}\ s^{-1}$	[20]
125	$Br_2 + O_2^{\bullet-} \rightarrow Br_2^{\bullet-} + O_2$	$5.6\times10^9\ M^{-1}\ s^{-1}$	[20]
126	$Br_2 + H_2O \rightarrow HOBr + Br^- + H^+$	$97\ M^{-1}\ s^{-1}$	[21]
127	$Br_2 + H_2O_2 \rightarrow 2HBr + O_2$	$1.3\times10^3\ M^{-1}\ s^{-1}$	[16]
128	$Br_3^- \rightarrow Br_2 + Br^-$	$5.5\times10^7\ s^{-1}$	[17]
129	$Br_3^- + HO_2^{\bullet} \rightarrow Br_2^{\bullet-} + HBr + O_2$	$1.0\times10^7\ M^{-1}\ s^{-1}$	[20]
130	$Br_3^- + O_2^{\bullet-} \rightarrow Br_2^{\bullet-} + Br^- + O_2$	$1.5\times10^9\ M^{-1}\ s^{-1}$	[20]
131	$HOBr + Br^- + H^+ \rightarrow Br_2 + H_2O$	$1.6\times10^{10}\ M^{-1}\ s^{-1}$	[22]
132	$HOBr + HO_2^- \rightarrow Br^- + H_2O + O_2$	$7.6\times10^8\ M^{-1}\ s^{-1}$	[17]
133	$HOBr + H_2O_2 \rightarrow HBr + H_2O + O_2$	$3.5\times10^4\ M^{-1}\ s^{-1}$	[23]
134	$HOBr + {}^{\bullet}OH \rightarrow BrO^{\bullet} + H_2O$	$2.0\times10^9\ M^{-1}\ s^{-1}$	[20]
135	$HOBr + O_2^{\bullet-} \rightarrow O_2 + OH^- + Br^{\bullet}$	$3.5\times10^9\ M^{-1}\ s^{-1}$	[24]

No	Reaction	Rate Constant	Reference
136	$HOBr + HO_2^{\bullet} \rightarrow BrOH^{\bullet-} + H^+$	3.5×10^9 M^{-1} s^{-1}	[18]
137	$BrO^- + H_2O_2 \rightarrow Br^- + H_2O + O_2$	1.2×10^6 M^{-1} s^{-1}	[17]
138	$BrO^- + {}^{\bullet}OH \rightarrow BrO^{\bullet} + OH^-$	4.5×10^9 M^{-1} s^{-1}	[17]
139	$BrO^-+O_2^{\bullet-}+H_2O\rightarrow Br^{\bullet}+2OH^- + O_2$	2.0×10^8 M^{-1} s^{-1}	[24]
140	$HOBr+SO_4^{\bullet-} \rightarrow BrO^{\bullet} + SO_4^{2-} + H^+$	2.0×10^9 M^{-1} s^{-1}	[23]
141	$BrO^- + SO_4^{\bullet-} \rightarrow BrO^{\bullet} + SO_4^{2-}$	4.5×10^9 M^{-1} s^{-1}	[23]
142	$BrO^{\bullet} + BrO^{\bullet} + H_2O \rightarrow$ $BrO^- + BrO_2^- + 2H^+$	5.0×10^9 M^{-1} s^{-1}	[17]
143	$BrO^{\bullet} + BrO_2^- \rightarrow BrO^- + BrO_2^{\bullet}$	3.4×10^8 M^{-1} s^{-1}	[17]
144	$Br_2^{\bullet-}+ BrO_2^-\rightarrow BrO^- + BrO^{\bullet} + Br^-$	8.0×10^7 M^{-1} s^{-1}	[17]
145	${}^{\bullet}OH + BrO_2^- \rightarrow BrO_2^{\bullet} + OH^-$	1.9×10^9 M^{-1} s^{-1}	[17]
146	${}^{\bullet}OH + BrO_2^{\bullet} \rightarrow BrO_3^- + H^+$	2.0×10^9 M^{-1} s^{-1}	[17]

No	Reaction	Rate Constant	Reference
147	$BrO_2^{\bullet} + BrO_2^{\bullet} \rightarrow Br_2O_4$	1.4×10^{9} M^{-1} s^{-1}	[17]
148	$Br_2O_4 \rightarrow BrO_2^{\bullet} + BrO_2^{\bullet}$	7.0×10^{7} s^{-1}	[17]
149	$Br_2O_4 + OH^{-} \rightarrow BrO_3^{-} + BrO_2^{-} + H^{+}$	7.0×10^{8} M^{-1} s^{-1}	[17]
150	$BrO_2^{\bullet} + BrO_2^{\bullet} + H_2O \rightarrow BrO_3^{-} + BrO_2^{-} + 2H^{+}$	4.2×10^{7} M^{-1} s^{-1}	[25]

Table S2. Modeled steady-state concentrations of $^{\bullet}OH$ and $SO_4^{\bullet-}$ in different water matrices.

Radical species (M)		Control[a]	Cl^- (mM)			HCO_3^- (mM)		
			0.5	1	3	0.5	1	3
ACY	$^{\bullet}OH$ ($\times10^{-14}$)	8.80	18.57	33.24	39.11	8.05	7.48	5.69
	$SO_4^{\bullet-}$ ($\times10^{-13}$)	7.56	4.52	3.24	1.52	7.08	7.46	5.71
ATL	$^{\bullet}OH$ ($\times10^{-14}$)	6.62	18.15	22.98	10.90	6.67	6.60	6.48
	$SO_4^{\bullet-}$ ($\times10^{-13}$)	5.70	4.39	1.49	1.38	4.33	4.11	3.77

[a] Conditions: $[ACY]_0$ = 0.022 mM, $[ATL]_0$ = 0.019 mM, PDS= 0.6 mM, UV_{254}, pH = 6.0, T = 20°C.

Table S3. Calculated condensed Fukui function and dual descriptor of ACY.[a]

Atom	q(N)	q(N+1)	q(N-1)	*f*-	*f*+	*f*0	CDD
1(C)	0.0627	0.0029	0.1251	0.0624	0.0597	0.0611	-0.0027
2(C)	-0.0286	-0.0838	0.0628	0.0914	0.0552	0.0733	-0.0362
3(C)	0.1549	0.1206	0.1953	0.0404	0.0343	0.0373	-0.0062
4(N)	-0.0773	-0.1292	-0.0517	0.0257	0.0519	0.0388	0.0262
5(C)	0.1586	0.0481	0.2092	0.0506	0.1105	0.0806	0.0599
6(N)	-0.2273	-0.2777	-0.1399	0.0873	0.0504	0.0689	-0.0369
7(N)	-0.0167	-0.0585	0.0112	0.0279	0.0417	0.0348	0.0138
8(C)	0.0495	-0.0132	0.1563	0.1068	0.0628	0.0848	-0.0440
9(N)	-0.1926	-0.2383	-0.1218	0.0708	0.0457	0.0583	-0.0251
10(C)	0.0907	0.0752	0.0984	0.0077	0.0155	0.0116	0.0077
11(O)	-0.1582	-0.1643	-0.1543	0.0039	0.0061	0.0050	0.0021
12(C)	0.0324	0.0229	0.0379	0.0055	0.0095	0.0075	0.0040
13(C)	0.0254	0.0149	0.0293	0.0039	0.0105	0.0072	0.0066
14(O)	-0.2398	-0.2601	-0.2273	0.0124	0.0203	0.0164	0.0079
15(O)	-0.3038	-0.3782	-0.1739	0.1299	0.0744	0.1021	-0.0556
16(N)	-0.1678	-0.2328	-0.0953	0.0725	0.0650	0.0688	-0.0074
17(H)	0.1417	0.1057	0.1698	0.0281	0.0360	0.0320	0.0079
18(H)	0.0605	0.0257	0.1048	0.0443	0.0348	0.0395	-0.0095
19(H)	0.0374	0.0113	0.0538	0.0164	0.0261	0.0213	0.0097
20(H)	0.0375	0.0205	0.0505	0.0131	0.0169	0.0150	0.0038
21(H)	0.0341	0.0232	0.0425	0.0084	0.0108	0.0096	0.0024
22(H)	0.0341	0.0246	0.0424	0.0082	0.0096	0.0089	0.0014
23(H)	0.0304	0.0215	0.0340	0.0036	0.0089	0.0063	0.0052
24(H)	0.0299	0.0221	0.0333	0.0033	0.0078	0.0056	0.0045
25(H)	0.1727	0.1356	0.1830	0.0103	0.0371	0.0237	0.0269
26(H)	0.1316	0.0935	0.1615	0.0299	0.0381	0.0340	0.0082
27(H)	0.0678	0.1630	0.0350	0.0603	0.0476	0.0253	0.021

[a] Units used above are “e” (elementary charge).

Table S4. Calculated condensed Fukui function and dual descriptor of ATL.[a]

Atom	q(N)	q(N+1)	q(N-1)	*f*-	*f*+	*f*0	CDD
1(O)	-0.3236	-0.3728	-0.2092	0.1144	0.0492	0.0818	-0.0652
2(C)	0.1648	0.1477	0.1971	0.0323	0.0171	0.0247	-0.0152
3(N)	-0.1540	-0.1679	-0.1237	0.0303	0.0140	0.0221	-0.0163
4(C)	-0.0516	-0.0643	-0.0304	0.0212	0.0127	0.0169	-0.0085
5(C)	-0.0166	-0.0515	0.0407	0.0573	0.0349	0.0461	-0.0224
6(C)	-0.0429	-0.1298	-0.0102	0.0326	0.0870	0.0598	0.0543
7(C)	-0.0566	-0.1662	-0.0069	0.0497	0.1095	0.0796	0.0598
8(C)	0.0760	0.0371	0.1268	0.0508	0.0389	0.0449	-0.0119
9(O)	-0.1262	-0.1458	-0.0543	0.0719	0.0196	0.0457	-0.0523
10(C)	0.0315	0.0233	0.0429	0.0114	0.0082	0.0098	-0.0032
11(C)	0.0443	0.0403	0.0478	0.0035	0.0040	0.0038	0.0005
12(O)	-0.2520	-0.2572	-0.2405	0.0115	0.0052	0.0083	-0.0063
13(C)	-0.0131	-0.0181	-0.0037	0.0094	0.0050	0.0072	-0.0045
14(N)	-0.1293	-0.1357	-0.0760	0.0533	0.0064	0.0299	-0.0469
15(C)	0.0288	0.0250	0.0359	0.0071	0.0038	0.0055	-0.0033
16(C)	-0.0943	-0.1017	-0.0831	0.0112	0.0075	0.0093	-0.0037
17(C)	-0.0888	-0.0967	-0.0824	0.0065	0.0079	0.0072	0.0014
18(C)	-0.0712	-0.1571	-0.0271	0.0441	0.0859	0.0650	0.0418
19(C)	-0.0453	-0.1485	-0.0049	0.0405	0.1032	0.0718	0.0627
20(H)	0.1177	0.1176	0.1285	0.0108	0.0001	0.0055	-0.0107
21(H)	0.1337	0.1128	0.1573	0.0236	0.0208	0.0222	-0.0028
22(H)	0.0473	0.0253	0.0708	0.0235	0.0220	0.0227	-0.0015
23(H)	0.0475	0.0232	0.0701	0.0226	0.0244	0.0235	0.0018
24(H)	0.0447	-0.0003	0.0691	0.0244	0.0450	0.0347	0.0206
25(H)	0.0491	-0.0019	0.0773	0.0281	0.0510	0.0396	0.0229
26(H)	0.0364	0.0261	0.0535	0.0171	0.0103	0.0137	-0.0068
27(H)	0.0303	0.0188	0.0469	0.0167	0.0115	0.0141	-0.0052
28(H)	0.0224	0.0150	0.0309	0.0086	0.0073	0.0080	-0.0013
29(H)	0.1284	0.1168	0.1403	0.0119	0.0115	0.0117	-0.0004
30(H)	0.0345	0.0297	0.0436	0.0091	0.0047	0.0069	-0.0044
31(H)	0.0225	0.0156	0.0386	0.0162	0.0069	0.0115	-0.0092
32(H)	0.1039	0.0888	0.1217	0.0178	0.0151	0.0165	-0.0027
33(H)	0.0320	0.0272	0.0401	0.0081	0.0048	0.0064	-0.0033
34(H)	0.0338	0.0195	0.0495	0.0157	0.0143	0.0150	-0.0013
35(H)	0.0292	0.0259	0.0328	0.0036	0.0033	0.0035	-0.0003
36(H)	0.0278	0.0193	0.0359	0.0081	0.0085	0.0083	0.0004
37(H)	0.0345	0.0217	0.0471	0.0125	0.0128	0.0127	0.0003
38(H)	0.0334	0.0269	0.0389	0.0055	0.0065	0.0060	0.0010
39(H)	0.0293	0.0208	0.0363	0.0070	0.0086	0.0078	0.0016
40(H)	0.0391	-0.0024	0.0635	0.0245	0.0415	0.0330	0.0171
41(H)	0.0426	-0.0066	0.0684	0.0257	0.0492	0.0375	0.0235

Table S5. Major intermediates of ACY detected in UV/PDS process.

TPs	Retention time(min)	Chemical Formula	Exact Mass	Identified method
ACY	1.645	$C_8H_{11}N_5O_3$	225.0	UPLC-Q-TOF-MS
TP1	4.554	$C_8H_{13}N_5O_4$	243.0	UPLC-Q-TOF-MS
TP2	4.754	$C_8H_{13}N_5O_5$	259.0	UPLC-Q-TOF-MS
TP3	1.296	$C_7H_{11}N_5O_4$	213.0	UPLC-Q-TOF-MS
TP4	5.019	$C_7H_{11}N_3O_4$	201.0	UPLC-Q-TOF-MS
TP5	5.684	$C_7H_{14} N_3O_4$	203.0	UPLC-Q-TOF-MS
TP6	1.345	$C_5H_7N_3O_3$	157.0	UPLC-Q-TOF-MS

Table S6. Major intermediates of ATL detected in UV/PDS process.

TPs	Retention time(min)	Chemical Formula	Exact Mass	Identified method
ATL	4.004	$C_{14}H_{22}N_2O_3$	266.2	UPLC-Q-TOF-MS
TP1	13.050	$C_{14}H_{21}NO_4$	267.1	UPLC-Q-TOF-MS
TP2	1.677	$C_{13}H_{19}NO_3$	237.1	UPLC-Q-TOF-MS
TP3	4.852	$C_{13}H_{19}NO_4$	253.1	UPLC-Q-TOF-MS
TP4	1.245	$C_6H_{15}NO_2$	133.1	UPLC-Q-TOF-MS
TP5	4.104	$C_{11}H_{16}N_2O_3$	224.1	UPLC-Q-TOF-MS
TP6	3.406	$C_8H_9NO_2$	151.0	UPLC-Q-TOF-MS
TP7	5.765	$C_{16}H_{16}N_2O_6$	332.0	UPLC-Q-TOF-MS
TP8	1.677	$C_{14}H_{22}N_2O_4$	282.1	UPLC-Q-TOF-MS
TP9	4.071	$C_{14}H_{20}N_2O_4$	280.1	UPLC-Q-TOF-MS
TP10	1.689	$C_{14}H_{22}N_2O_5$	298.1	UPLC-Q-TOF-MS

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