Supplementary Information

for

Effects of UV/PMS oxidation on the degradation of zidovudine： kinetics, degradation products, and reaction pathways

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Contents

Test S1. Methods of analysis

1. Detection methods for routine indicators

The main conventional indicators involved in this study include turbidity, pH, conductivity, UV_{254}, hardness, nitrate-nitrogen, nitrite-nitrogen, sulfate, chloride, ammonia nitrogen, total organic carbon (TOC), and dissolved organic carbon (DOC). Among them, TOC is directly detected by a Shimadzu TOC analyzer. For DOC detection, the water samples need to be filtered through a 0.45-μm filter membrane before being analyzed using the instrument. The pH value is measured by an FE28 pH meter. The detection of UV_{254} is carried out using a UV-2700 UV spectrophotometer. The turbidity value is obtained by a 2100N turbidimeter. Conductivity is detected with a DDS-307A conductivity meter. Nitrate-nitrogen, nitrite-nitrogen, sulfate, chloride, and ammonia nitrogen are determined according to Methods for Monitoring and Analyzing Water and Wastewater (please specify the edition number). The detection of hardness (expressed as $CaCO_3$) refers to Standard Test Methods for Drinking Water (GB/T 5750.4 - 2006).

2. Determination of AZT and its products

(1) Preparation of AZT stock solution

An appropriate amount of AZT standard (purity ≥ 98%, determined by HPLC) was accurately weighed and dissolved in Milli-Q ultrapure water. After stirring until fully dissolved, the solution was diluted to the required concentration to prepare a stock solution. This stock solution was stored in amber containers (to protect against light exposure, as AZT is photosensitive) and refrigerated at 4°C for subsequent use.

(2) Detection methods

The concentration of AZT was determined using a Waters Acquity Arc high-performance liquid chromatograph. The chromatographic column model was InerSustain C18 (4.6 mm × 250 mm, 5 μm). The separation speed of the chromatographic column was 0.5 $mL \cdot min^{-1}$, and the column temperature was 25 °C. Methanol and water were used as the mobile phase in a ratio of 40:60. The detection wavelength was set at 265 nm, and the injection volume was 10 μL. The retention time of AZT was 7.3 min.

The degradation products of AZT were determined using an Agilent ultra-high-pressure liquid

chromatography-quadrupole time-of-flight mass spectrometer. The flow rate was set at 0.3 mL·min^{-1}, and the injection volume was 5 μL. The chromatographic column was Waters BEH C18 (2.1 × 100 mm, 1.7 μm). Mobile phase A was a 0.1% formic acid aqueous solution, and mobile phase B was an acetonitrile solution. The ratio of mobile phase A to mobile phase B was 9:1 from 0 to 2 min, 0:100 from 15 to 20 min, and 9:1 from 21 to 30 min. The mass spectrometry scanning range for the first stage was 50–500 m/z. The sheath gas temperature was 350 °C, the sheath gas flow rate was 12 L·min^{-1}, and the voltage was 4000 V.

3. Determination of nitrobenzene (NB) concentration

(1) Pretreatment

In the section on determining the secondary reaction rates of $SO_4^{\bullet-}$ and $OH^{\bullet}$ with AZT, NB is required as a free radical probe [1]. During the experiment, at six time points (0, 11.85, 23.68, 35.53, 47.38, and 59.23 min), 100 mL of the reaction solution was completely transferred to amber glass bottle, and 1 mL of $Na_2S_2O_3$ solution was added each time. A total of six experiments were conducted, resulting in six bottles of 101 mL of the solution to be extracted. In this study, a fully automated solid-phase extractor was used to replace the aqueous solvent of the NB samples to be tested with dichloromethane (CH_2Cl_2) to facilitate gas-phase detection. The extraction columns used were HLB-type adsorbent columns (6 cc/200 mg, 30 μm) manufactured by Waters, which are disposable columns. The main process of solid-phase extraction is as follows: The extraction column was activated sequentially with 10 mL of CH_2Cl_2 and 5 mL of ultrapure water. Then, 101 mL of the solution to be extracted was loaded onto the instrument at a flow rate of 6 mL·min^{-1}. Subsequently, the extraction column was rinsed with 10 mL of ultrapure water. After nitrogen stripping for 20 min, 5 mL of CH_2Cl_2 was used for elution, and the concentrated solution was collected. Finally, a nitrogen blowing instrument was used to concentrated to near dryness, and it was then dissolved to a volume of 5 mL with CH_2Cl_2. The solution was placed in a refrigerator at 4 °C, and the determination was completed within 24 h.

(2) Gas chromatography

The NB concentration in the solution to be tested was detected using an Agilent 7890A gas chromatograph. The chromatographic column was an HP - 5.5% Phenyl Methyl Siloxan capillary column (30 m × 320 μm × 0.25 μm). The carrier gas was nitrogen. Split injection was adopted with

a split ratio of 5:1. The split flow rate was 5 mL·min^{-1}, the septum purge flow rate was 3 mL·min^{-1}, and the make-up gas flow rate was 60 mL·min^{-1}. The initial temperature of the column oven was 100 °C and was maintained for 2 min. Then, the temperature was increased to 200 °C at a rate of 10 °C·min^{-1} and maintained for 4 min. The temperatures of the injection port and the detector were 240 °C and 330 °C, respectively.

4. Determination of atrazine (ATZ) concentration

(1) Pretreatment

In the section on determining the secondary reaction rate of $SO_4^{\bullet-}$ and AZT, ATZ is required as a free radical probe. During the experiment, at six time points (0, 11.85, 23.68, 35.53, 47.38, and 59.23 min), 100 mL of the reaction solution was completely taken out and transferred to brown reagent bottles, and 1 mL of $Na_2S_2O_3$ solution was added respectively. A total of six experiments were carried out, resulting in six bottles of 101 mL of the solution to be extracted.

In this study, a fully automated solid-phase extractor was used to replace the aqueous solvent of the NB samples to be tested with dichloromethane (CH_2Cl_2) to facilitate gas-phase detection. The extraction column used was the HLB-type adsorbent column (6 cc/200 mg, 30 μm) produced by Waters. The main process of solid-phase extraction was as follows: The extraction column was activated sequentially with 5 mL of CH_2Cl_2 and 5 mL of ultrapure water. Then, 101 mL of the solution to be extracted was loaded onto the instrument at a flow rate of 6 mL·min^{-1}. Subsequently, the extraction column was rinsed with 10 mL of ultrapure water. After nitrogen stripping for 20 min, 5 mL of CH_2Cl_2 was used for elution and the concentrated solution was collected. The concentrated solution was blown to a trace amount using a nitrogen blowing instrument and then diluted to 5 mL with CH_2Cl_2. The solution was placed in a refrigerator at 4 °C, and the determination was completed within 24 h.

(2) Gas chromatography

The concentration of ATZ in the solution to be tested was detected using a Thermo Fisher Trace DSQ gas chromatography-mass spectrometry (GC-MS) instrument. the gas chromatographic column was an HP-5MS capillary column was HP-5MS (30 m × 0.25 mm, 0.25 μm). The carrier gas flow rate was set at 1 mL·min^{-1}, and splitless injection was used. The temperature of the injection port was 230 °C, and the injection volume was 1.0 μL. The temperature programming was as

follows: The initial temperature was set at 45 °C and maintained for 1.0 min. Then, the temperature was increased to 130 °C at a rate of 40 °C·min^{-1}, followed by an increase to 180 °C at a rate of 12 °C·min^{-1}. Finally, the temperature was increased to 240 °C at a rate of 7 °C·min^{-1} and maintained for 3 min. For the mass spectrometry conditions, the temperatures of the ion source and the interface were 230 °C and 260 °C, respectively. The selected ion monitoring (SIM) mode was set, and the mass-to-charge ratios (m/z) of the quantitative ions were 95, 112, 200, and 215, respectively. The solvent delay was 4.4 min.

5. Detection of natural organic matter

The separation and qualitative analysis of natural organic matter were carried out with a liquid chromatography-organic carbon detector (LC-OCD), a large-scale water quality analysis instrument developed by Dr. Stefan Huber (Germany). The detection principle relies on the separation of the molecular weights of organic matter by size exclusion chromatography. In addition to the OCD detector, a ultraviolet detector (UVD) with a wavelength of 254 nm and an organic nitrogen detector (OND) can be added to the equipment for the detection of corresponding indicators. During the detection, each sample takes 70 minutes, and the injection volume is set at 1000 uL. Finally, data were calculated using the instrument's proprietary software, followed by manual integration to obtain the detection results.

6. Detection of fluorescent organics

Fluorescent organic matter was detected using a three-dimensional excitation-emission matrix (3D-EEM) fluorescence spectrometer, whose full English name is Excitation Emission Matrix Spectra. It is widely used in the detection of fluorescent components in samples such as natural water bodies and wastewater effluents [2]. The F-2700 instrument manufactured by Hitachi Company of Japan was used for the detection. During the detection, 50 mL of the sample was first taken and filtered through a 0.45 μm membrane filter. After thorough mixing, an appropriate volume of the filtrate was transferred to a quartz cuvette, which was then put into the instrument. The widths of the excitation and emission slits were set to 5 nm and 3 nm, respectively. The ranges of excitation and emission were set to 200–450 nm and 200–550 nm, respectively. The scanning speed was set to 1200 nm·min^{-1}, and the interval was 5 nm for both. After the detection was completed, the 3D-EEM spectra were processed using Origin software.

7. Sterilization by-product precursor testing

The detection of disinfection byproduct precursors determined by the total yield of the corresponding disinfection byproducts in the water body after adding sufficient chlorine to the water sample and allowing it to react for a sufficient time [3]. Before chlorination, the pH value of the water sample needs to be adjusted to 7.0 ± 0.2 with a phosphate buffer solution. Take 30 mL of the water sample into a brown bottle, and sodium hypochlorite was added at 3–5 times the TOC concentration of the water sample of the water sample, so that the concentration of free residual chlorine is in the range of 3–5 $mg \cdot L^{-1}$ at the end of chlorination . After the water sample is shaken well, it is placed in an incubator at 25 °C in a dark environment for incubated at 25 °C in the dark with the following reaction times. The chlorination time for the precursors of trihalomethanes (THMs) is 72 h, and the chlorination times for the precursors of haloacetic acids (HAAs), haloacetonitriles (HANs), and halonitromethanes (HNMs) are all 24 h. At the end of chlorination, pre-weighed excess ascorbic acid was rapidly added to quench residual chlorine to the brown bottle, and the bottle is capped and shaken well.

(1) For the detection of the precursors of trihalomethanes (THMs), the instrument used to detect the THMs generated in the water sample is the Shimadzu GC-2010 gas chromatograph. Analysis was performed according to GB/T 5750.8 - 2006. 10 mL of sample was added to headspace vials used for detection is 10 mL. Chromatographic column: HP-5 capillary column column (30.0 m × 0.32 mm × 0.25 μm), and the column flow rate is set at 1.0 $mL \cdot min^{-1}$. The temperature of the injection port is 220 °C, the carrier gas is nitrogen, and the purge flow rate is 3 $mL \cdot min^{-1}$. The injection mode is split, with a split ratio of 30.0 and a linear velocity of 18.5 $cm \cdot sec^{-1}$, and the total flow rate is 34.1 $mL \cdot min^{-1}$. Detector temperature: 300 °C, and the make - up gas flow rate is 30 $mL \cdot min^{-1}$. Oven temperature program: The initial temperature is 35 °C and held for 5 min. Then, the temperature is increased to 50 °C at a rate of 1 $°C \cdot min^{-1}$ and maintained for 12.5 min. The total sample measurement time is 32.5 min.

(2) HAA precursors in water samples were analyzed using a Waters Xevo TQ-S ultra-performance liquid chromatography-tandem mass spectrometer (UPLC-MS/MS), with an injection volume of 1 mL in 2-mL autosampler vials. The chromatograph was equipped with an ACQUITY UPLC HSS T3 column (1.8 μm, 2.1 mm × 100 mm). The mobile phases were acetonitrile (A) and

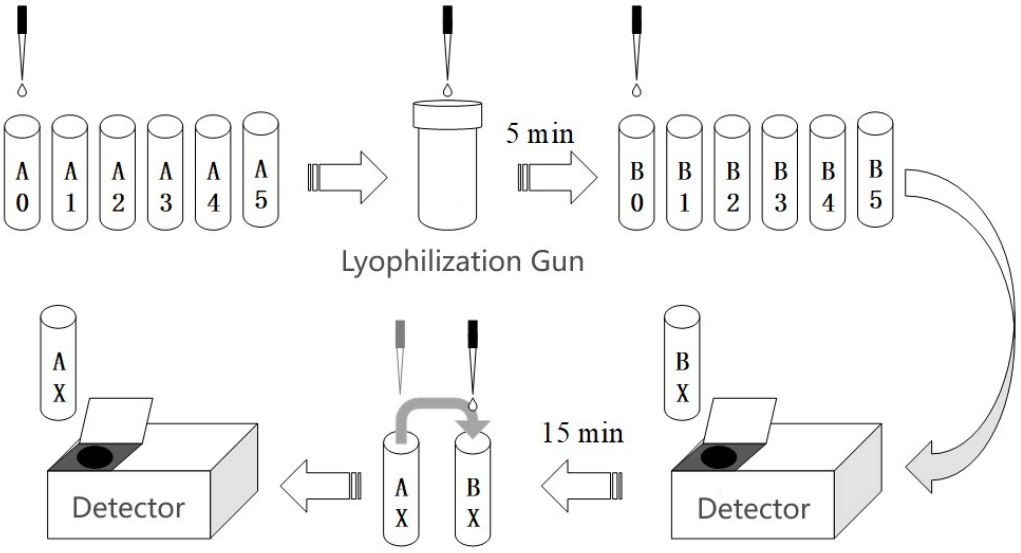
0.05% formic acid in water (B). The mobile phase gradient was as follows: initially, A:B = 2:98; 3.0–3.5 min: 20% A, 80% B; from 4.5 min, A:B = 90:10; from 6 min, A:B = 2:98. The flow rate was 0.4 $mL \cdot min^{-1}$, and the temperatures of the sample and the column were 10.0 °C and 30.0 °C, respectively. For the mass spectrometry conditions, the ionization mode was ES^-, the source temperature was 150 °C, the desolvation gas temperature was 600 °C, the cone gas flow rate was 150 $L \cdot h^{-1}$, the desolvation gas flow rate was 1000 $L \cdot h^{-1}$, and the nebulizer pressure was 7.0 Bar.

(3) Haloacetonitriles (HANs), Halogenated Nitromethane (HNMs) Precursors

For HAN and HNM precursor analysis, chlorinated water samples were quenched, and the pH was adjusted to 4.0. Subsequently, 1 g of anhydrous sodium sulfate, 10 mL of the aqueous sample, and 1 mL of methyl tert-butyl ether (MTBE) extractant were sequentially added to headspace vials, ensuring equal volumes of the aqueous and organic phases. Standard solutions were processed identically. The instrument used to detect the THMs and HNMs generated was the TQ8040 triple quadrupole gas chromatography-mass spectrometer manufactured by Shimadzu Corporation.

The chromatographic column used was Rtx - 5MS (60 m × 0.25 mm × 2.5 μm). The column flow rate was 1.2 $mL \cdot min^{-1}$. The injection mode was splitless injection, and the injection volume was 1 μL. The carrier gas was high - purity helium. The temperature programming was as follows: Initially, the temperature was maintained at 40 °C for 5 min. Then, the temperature was increased to 80 °C at a rate of 5 $°C \cdot min^{-1}$ and maintained for 2 min. Finally, the temperature was increased to 180 °C at a rate of 40 $°C \cdot min^{-1}$ and held for 3 min. For the mass spectrometry conditions, the ion source mode was EI (70 eV). The temperatures of the ion source, the injection port, and the transfer line were 200 °C, 170 °C, and 200 °C, respectively. The solvent delay time was 6.8 min. The detector voltage was the tuning voltage + 0.4 kV. The scanning mode was set to the selected ion monitoring (SIM) mode.

8. Acute toxicity testing



Comprehensive Toxicity Testing Flowchart

Vibrio fischeri was employed to assess toxicity changes in solutions during AZT degradation by UV/PMS technology. The standards followed in the measurement process include the standards of the American Society for Testing and Materials (ASTM-D-5660) and the standards of the European Committee for Standardization (EN ISO 11348 - 3 - 2008), etc. The instrument used for the detection was GR-8500A portable toxicity analyzer. Before starting, the instrument was powered on and preheated for 60 s. The specific steps involved are shown in the figure.

(1) 1 mL of diluent and 0.1 mL of osmotic pressure adjusting solution were pipetted into tube A0. Then, add 1 mL of the corresponding water sample and 0.1 mL of the osmotic pressure regulating solution to tubes A1–A5 in sequence.

(2) Lyophilized *Vibrio fischeri* powder and diluent were removed from the freezer and refrigerator, respectively and the refrigerated layer of the refrigerator, respectively. Use a pipette to add 3.5 mL of the diluent to the vial containing the lyophilized powder. After mixing well, carry out a resuscitation procedure that takes 5 minutes. Then, take 0.5 mL of the rehydrated solution after resuscitation and add it to bottles B0–B5, respectively.

(3) On the instrument, click on the more accurate B-TOX mode. Detect the luminescence intensity of the bacteria in bottles B0–B5 respectively. After the detection is completed, click the "Finish" option, and the instrument will automatically start timing for 15 minutes.

(4) During the waiting period, use a pipette to take 0.5 mL of the liquid from the AX bottle

(where X corresponds to the numbers 0–5) and add it to the BX bottle.

(5) After the 15–minute timing is over, put B0–B5 into the instrument for detection respectively.

(6) Query the test results and record them.

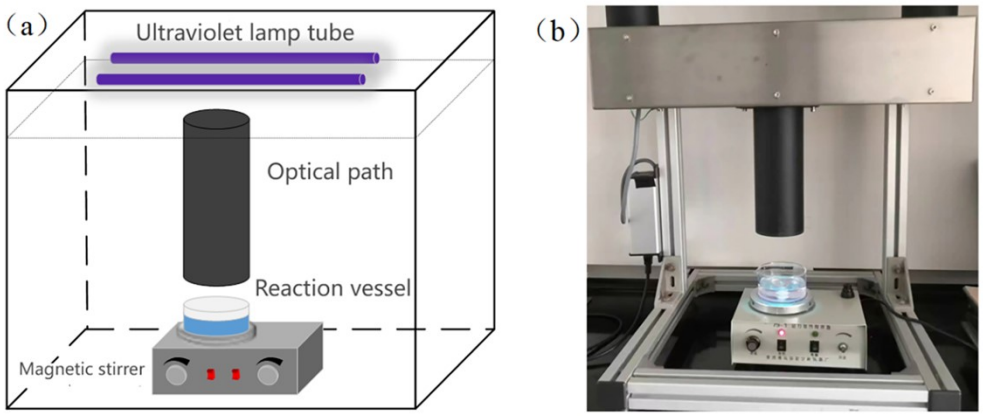
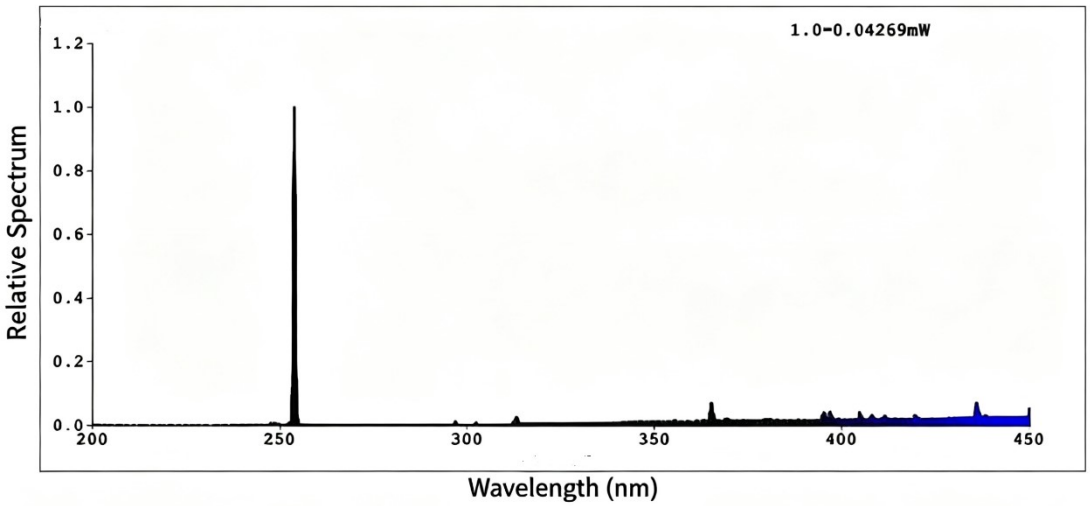


Figure S1. Schematic (a) and photographic (b) drawings of parallel beam device.



Peak Wavelength: λp = 253.8 nm Half-Width: λd = 0.9 nm

Figure S2. Light Source Spectral Test Report

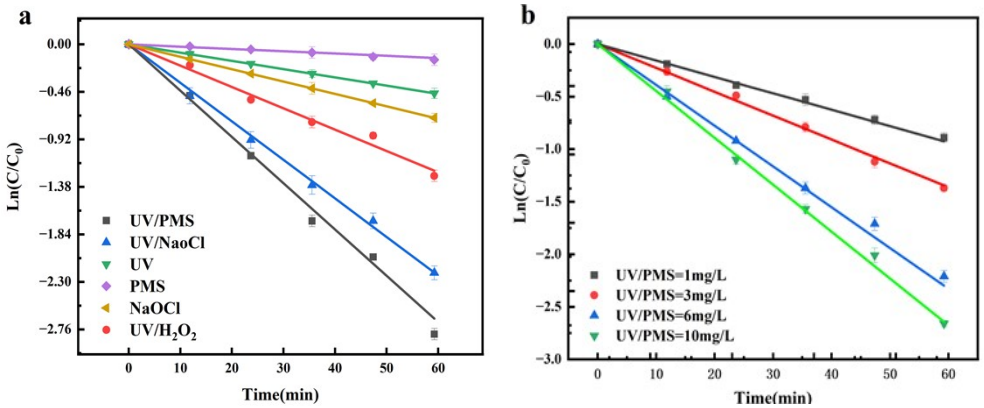


Figure S3. Quasi-primary fitting curves of AZT degradation by different UV advanced oxidation techniques and quasi-primary fitting curves of AZT degradation under UV/PMS system.

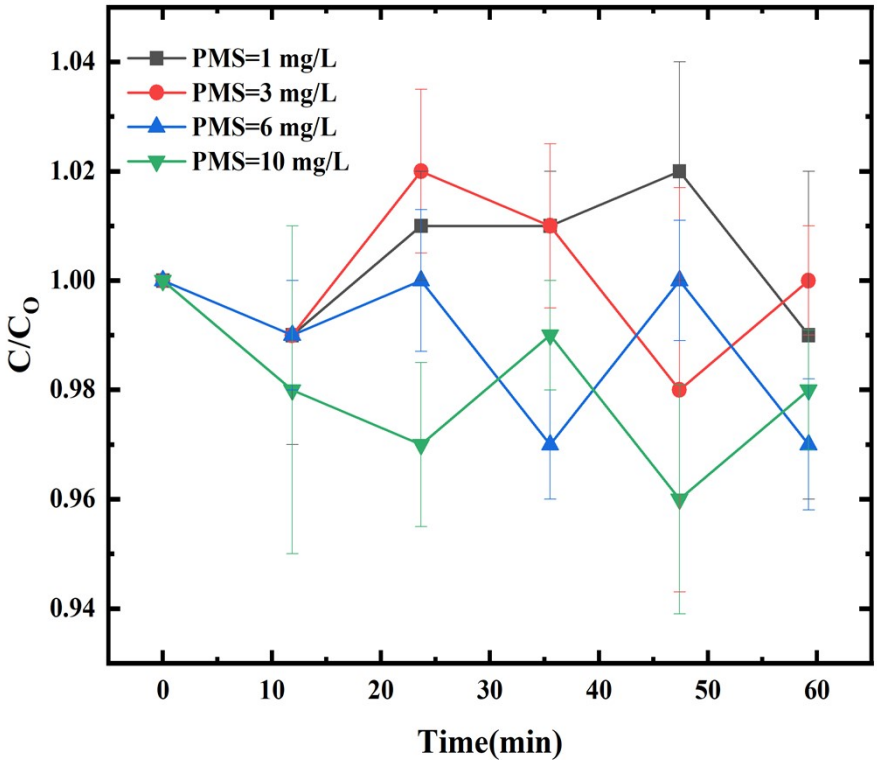


Figure S4. Removal of AZT in the PMS system

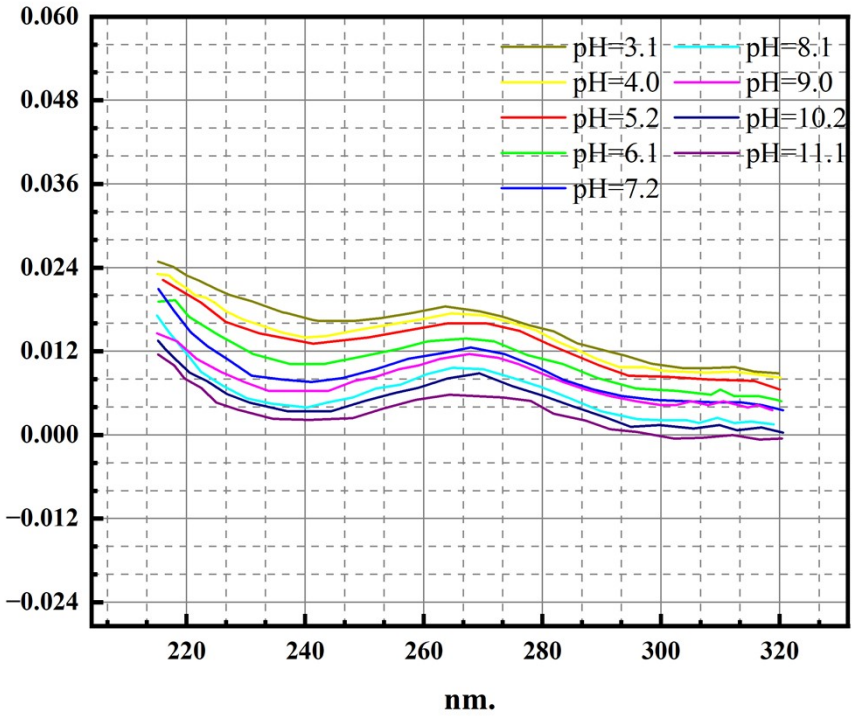
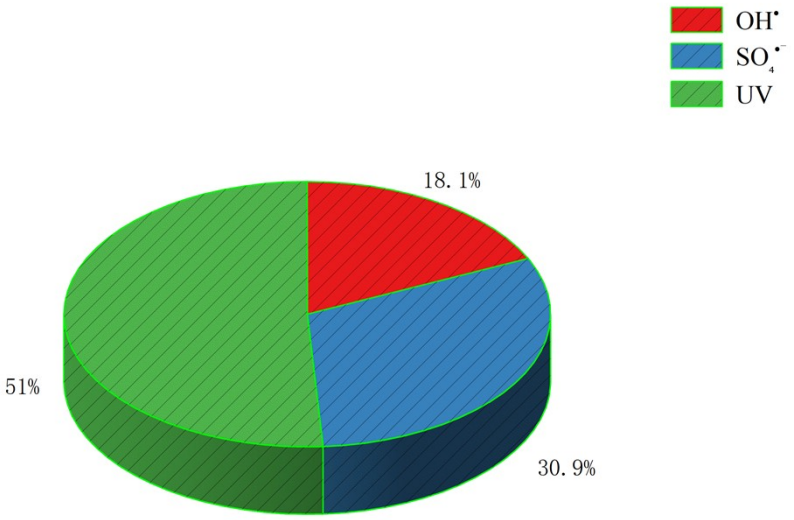


Figure S5. Variation of AZT absorbance at different pH with wavelength λ



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307 **Figure S6.** Contribution of $SO_4^{\bullet-}$, $OH^{\bullet}$, and UV to AZT degradation in UV/PMS systems

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Table S1. Degradation rates of 4-MBC and EHMC by different advanced oxidation processes.

Process Type	Target Pollutants	Degradation Efficiency
UV/PMS	4-MBC/EHMC	Ultra-pure water: 98% (EHMC, 200 mJ/cm²); Natural water: 92% (EHMC, 0.3 mM PMS)
UV/H_2O_2	4-MBC/EHMC	Ultra-pure water: 93% (EHMC); Natural water: 79% (0.3 mM H_2O_2)
UV/PMS/H_2O_2	4-MBC/EHMC	Ultra-pure water: 98% (synergistic effect); Natural water: 74% (0.015 mM mixture)
UV (control)	4-MBC/EHMC	Ultra-pure water: 53%; Natural water: 45% (1400 mJ/cm²)

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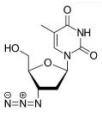
347 **Table S2.** Experiment main target organic matter

Name	Molecular weight	Chemistry	Norm	Provider	Dissociation Constant	logKow	Water Solubility
Zidovudine (AZT)	(267.24)		≥98% (HPLC)	Aladdin Reagent (Shanghai) Co.	$pKa_1 \approx 2.6–2.8$ $pKa_2 \approx 9.5–10.0$	≈ 0.05	20 mg/mL （25℃）

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350 **Table S3.** Experimental reagents

Name of experimental reagents	Specification/Model	Note
Potassium peroxymonosulfate complex salt ($2HKSO_5 \cdot KHSO_4 \cdot K_2SO_4$)	42%~46% ($KHSO_5$ metering)	Shanghai Eon Chemical Technology Co.
Disodium hydrogen phosphate dodecahydrate ($Na_2HPO_4 \cdot 12H_2O$)	Analytical purity	Aladdin Reagent (Shanghai) Co.
Sodium dihydrogen phosphate dihydrate ($NaH_2PO_4 \cdot 2H_2O$)	Analytical purity	Aladdin Reagent (Shanghai) Co.
Sodium thiosulfate ($Na_2S_2O_3$)	Analytical purity	Tianjin Komeo
Hydrogen peroxide (H_2O_2）	30%	Shanghai Guoyao
Sodium hypochlorite (NaClO)	22%	Tianjin Komeo
Sodium chloride (NaCl)	Analytical purity	Tianjin Komeo
Sodium bicarbonate ($NaHCO_3$)	Analytical purity	Tianjin Komeo
Sodium nitrate ($NaNO_3$)	Analytical purity Analytical purity	Shanghai Guoyao
Sodium Nitrite ($NaNO_2$)	Analytical purity	Shanghai Guoyao
Humic acid (HA)	≥90%	Aladdin Reagent (Shanghai) Co.
Methanol (CH_3OH)	Chromatographic purity	Merck KGaA
Trihalomethane standard	Chromatographic purity	TEDIA
Haloacetonitrile standard product	Chromatographic purity	AccuStandard
Haloacetic acid standard product	Chromatographic purity	Sigma-Aldrich
Halonitromethane standard product	Chromatographic purity	AccuStandard
Ascorbic acid ($C_6H_8O_6$)	Analytical purity	Shanghai Guoyao

Name of experimental reagents	Specification/Model	Note
Sodium hydroxide (NaOH)	Analytical purity	Shanghai Guoyao
Sulfuric acid (H_2SO_4)	Analytical purity	Shanghai Guoyao
Sodium sulfate anhydrous (Na_2SO_4)	Analytical purity	Shanghai Guoyao
Methyl tert-butyl ether ($C_5H_{12}O$)	Analytical purity	Shanghai Guoyao
Tert-butyl alcohol ($C_4H_{10}O$)	Chromatographic purity	Aladdin Reagent (Shanghai) Co.
Isopropyl alcohol (C_3H_8O)	Chromatographic purity	Aladdin Reagent (Shanghai) Co.
Nitrobenzene ($C_6H_5NO_2$)	Chromatographic purity	Aladdin Reagent (Shanghai) Co.
Atrazine ($C_8H_{14}ClN_5$)	Chromatographic purity	Aladdin Reagent (Shanghai) Co.
Dichloromethane (CH_2Cl_2)	Chromatographic purity	Merck KGaA
Formic acid (CH_2O_2)	Chromatographic purity	Aladdin Reagent (Shanghai) Co.
Acetonitrile (CH_3CN)	Chromatographic purity	Merck KGaA
Vibrio fischeri lyophilized powder	LS100-QF100	Beijing Zhongxi Yuanda Technology Co.

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352 **Table S4.** Main instruments and equipment

Instruments or equipment	Model number	Manufacturer
High Performance Liquid Chromatography	Waters Acquity Arc	Waters Corporation
Constant Temperature Magnetic Stirrer	85-2	Changzhou Guohua Electric
Gas Chromatograph	GC2010	Shimadzu, Japan
Gas Chromatograph	7890A	Agilent, USA
Gas Chromatography-Mass Spectrometer	Trace DSQ	Thermo Fisher Scientific
Triple Quadrupole Gas Chromatograph-Mass Spectrometer	TQ8040	Shimadzu, Japan
Ultra High Pressure Liquid Chromatography-Quadrupole Tandem Time of Flight Mass Spectrometer	1290UPLC /QTOF6550	Agilent, USA

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Instruments or equipment	Model number	Manufacturer
Total Organic Carbon Tester	TOC-VCPH	Shimadzu Corporation, Japan
Ultra High Performance Liquid Chromatography-Triple QuadrupoleMass Spectrometer	XevoTQ-S	Waters Corporation, USA
Portable H2O2 Concentration Detector	GDYS-102SC	Changchun Jida Swan Instrument Co.
Liquid Phase Organic Carbon Analyzer	LC-OCD	DOC-Labor Corporation
Fluorescence Excitation-Emission Matrix Spectrometer	F-2700	Hitachi, Japan
Ultraviolet irradiation	ILT 2400	International Light

intensity meter		Technologies, USA
Portable Residual Chlorine Meter	AQ3070	ThermoFisher, USA
Electronic Analytical Balance	MS204S/01	Mettle Toledo, Switzerland
Automatic Solid Phase Extractor	Auto SPE 06PLUS	China Ruike Instrument Co.
pH meter	FE28	Mettle Toledo, Switzerland
Turbidity meter	2100N	Hash Corporation, USA
Conductivity meter	DDS-307A	Shanghai Lei Magnetic Instrument Factory, China
UV Spectrophotometer	UV-2700	Shimadzu Corporation, Japan
Portable Comprehensive Toxicity Tester	GR-8500A	Hangzhou Lujie Water Technology Co.
Digital Blast Drying Oven	DDS-307A	Shanghai Lei magnetic Instrument Factory, China

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355 **Table S5.** L16(42)Orthogonal design and results table

	A:PMS concentration	B:UV dose	A*B	Removal rate
1	1 (1 mg·L^{-1})	1(200 mJ·cm^{-2})	1	32.29%
2	1	2(300 mJ·cm^{-2})	2	41.14%
3	1	3(400 mJ·cm^{-2})	3	47.68%
4	1	4(500 mJ·cm^{-2})	4	58.93%
5	2 (3 mg·L^{-1})	1	2	38. 74%
6	2	2	1	54.62%
7	2	3	4	67.37%
8	2	4	3	74.59%
9	3 (6 mg·L^{-1})	1	3	60.15%
10	3	2	4	74.59%
11	3	3	1	81.91%
12	3	4	2	89.03%
13	4 (10 mg·L^{-1})	1	4	66.80%
14	4	2	3	79.29%
15	4	3	2	86.59%
16	4	4	1	92.99%
K_1	45.01	49.50		
K_2	58.83	62.41		
K_3	76.42	58.62		
K_4	81.42	78.89		
R	36.41	29.39		

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Table S6. Water quality parameters of filtered water effluent

Water quality parameters (units)	Filtered water
Temperature（℃）	23
pH	8.27
UV_{254} (cm^{-1})	0.031
DOC($mg \cdot L^{-1}$)	2.205
Turbidity（NTU）	0.206
Total hardness (as $CaCO_3$)（$mg \cdot L^{-1}$）	239
Electrical conductivity（$\mu s \cdot cm^{-1}$）	886
Ammonia nitrogen（$mg \cdot L^{-1}$）	0.06
Nitrate (as N)（$mg \cdot L^{-1}$）	2.06
Nitrite (as N)（$mg \cdot L^{-1}$）	<0.005
Chloride（$mg \cdot L^{-1}$）	97.1
Sulfate（$mg \cdot L^{-1}$）	209

Table S7. Degradation products

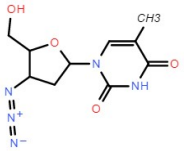
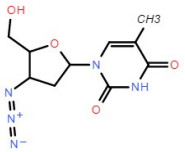
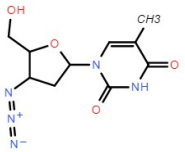
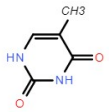
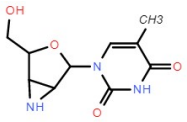
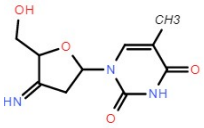
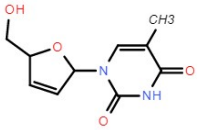
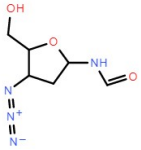
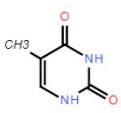
Nicknames	Mass-to-charge ratio measurements	Theoretical value of mass-to-charge ratio	Misalignment(ppm)	Predicting the original structure
AZT-1	268.1053	268.1040	4.85	
AZT-2	290.0872	290.0860	4.14	
AZT-3	306.0608	306.0599	2.91	
DP127	127.0510	127.0502	6.30	
DP239(a)	239.0916	239.0912	1.67	
DP239(b)	239.0916	239.0912	1.67	
DP223	223.0725	223.0724	0.45	
DP185	185.0667	185.0680	-7.02	
DP125	125.0355	125.0357	-1.6	

Table S8. Signal intensity

Nicknames	0 min Abund （Counts）	30 min Abund （Counts）	60 min Abund （Counts）
AZT-1	247961	89253	34438
AZT-2	28658	9876	4073
AZT-3	3395	1124	529
DP127	Not observed	678	1356
DP239(a)	Not observed	1239	979
DP239(b)	Not observed	1187	921
DP223	Not observed	19188	1789
DP185	Not observed	539	1338
DP125	Not observed	1338	2676

405 **Table S9.** Toxicity classifications and ranges (based on GHS)

Toxicity range ($mg \cdot L^{-1}$)	Hierarchy
$LC_{50}/EC_{50}/ChV \leq 1$	Extremely toxic
$1 < LC_{50}/EC_{50}/ChV \leq 10$	Toxic
$10 < LC_{50}/EC_{50}/ChV \leq 100$	Harmful
$LC_{50}/EC_{50}/ChV > 100$	Harmless

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Table S10. AZT and its products log KOW, acute toxicity, chronic toxicity assessment values (based on ECOSAR software)

	log KOW	Acute toxicity：mg·L^{-1}			Chronic toxicity：mg·L^{-1}		
		Fish (LC_{50})	Flea (LC_{50})	Chlorella (EC_{50})	Fish (ChV)	Flea (ChV)	Chlorella (ChV)
AZT	-7.051	3.67×10^{6}*	7.3×10^{9}*	0.020	2.71×10^{4}	4.93×10^{5}	0.005
DP239 (a)	-2.331	114.011	1126.008	0.018	12.514！	90.825！	0.005
DP239 (b)	-1.295	2017.275	16193.001	0.018	14.609	78.073	0.005
DP223	-0.791	19.295	4742.681	0.017	2.690！	34.310	0.005
DP185	-8.087	9.14×10^{8}*	3.95×10^{10}*	3.26×10^{6}*	38896.162	7.56×10^{6}*	43481.133
DP125	-0.32	383.824	901.557	0.009	2.193	9.552	0.003

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