Supplementary Material

A comparative study on the degradation of iohexol and diatrizoate during UV/persulfate process: kinetics, degradation pathways and disinfection by-products

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This document contains 1 Text, 5 Figures, and 2 Tables.

Text S1 Determination of the second-order rate constants of radicals with iohexol and diatrizoate

The concentration of benzoic acid (BA) was analyzed using an Agilent 1200 infinity series HPLC equipped with an XterraR MS C18 chromatographic column (250 mm $\times$ 2.1 mm, 3.5 μm, Waters, USA). The mobile phase was methanol and ultra-pure water at a ratio of 50%/50% (v/v) with the flow rate of 1.0 mL/min.

Competition kinetic approaches were applied to determine the second-order rate constants of HO• and SO_4^-• with iohexol and diatrizoate, using BA as the competitor (Ma et al., 2021). The concentrations of iohexol, diatrizoate, and BA were both 10 μM, and the dosages of H_2O_2 and PS were both 200 μM. 10 mM TBA was added in the solution to eliminate HO• in the UV/PS system. The k_{app} of SO_4^-• and HO• with ICM (iohexol or diatrizoate), $k_{SO_4^-•,ICM}$ and $k_{HO•,ICM}$, $M^{-1}s^{-1}$, are expressed in Eqs. (S1) and (S2):

$$k_{SO_4^-•,ICM} = \frac{k_{obs,UV/PS,ICM} - k_{obs,UV,ICM}}{k_{obs,UV/PS,BA}} \times k_{SO_4^-•,BA} \tag{S1}$$

$$k_{HO•,ICM} = \frac{k_{obs,UV/H_2O_2,ICM} - k_{obs,UV,ICM}}{k_{obs,UV/H_2O_2,BA}} \times k_{HO•,BA} \tag{S2}$$

where $k_{obs,UV/PS,ICM}$, $k_{obs,UV,ICM}$, and $k_{obs,UV/H_2O_2,ICM}$ are the pseudo first-order rate constant (s^{-1}) for ICM (iohexol or diatrizoate) in UV/PS, UV, and UV/H_2O_2 processes,respectively; $k_{obs,UV/PS,BA}$ and $k_{obs,UV/H_2O_2,BA}$ are the pseudo first-order rate constant (s^{-1}) for BA in UV/PS and UV/ H_2O_2 degradation, respectively. $k_{SO_4^-•,BA}$ and $k_{HO•,BA}$ are the second-order rate constants ($M^{-1}s^{-1}$) for SO_4^-• and HO• with BA, respectively, with values of 1.2×10^9 $M^{-1}s^{-1}$ and 5.9×10^9 $M^{-1}s^{-1}$, respectively (Lee et al., 2019).
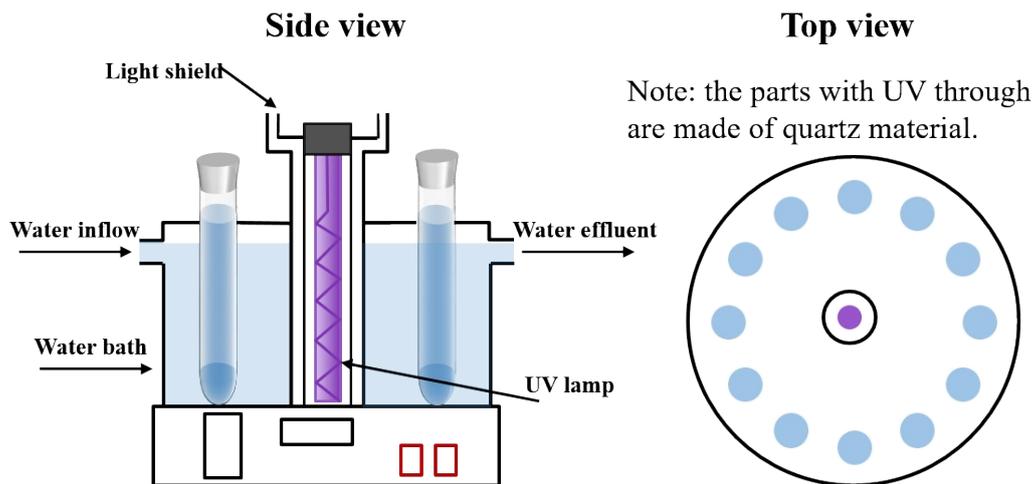
Figure S1 The schematic diagram of the photochemical reactor.
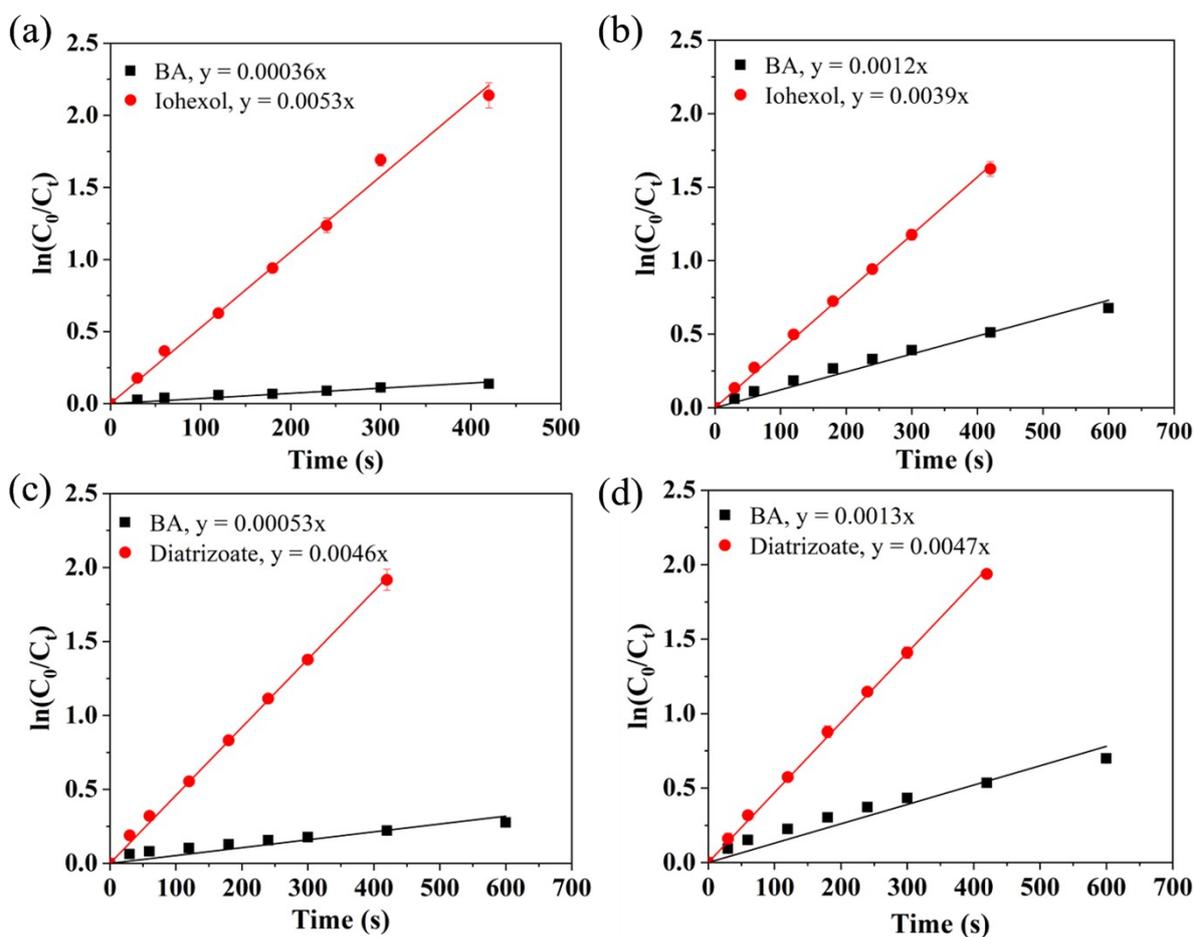
**Figure S2** Determination of the second-order rate constants of $SO_4^-\bullet$ ((a), (c)) and $HO\bullet$ ((b), (d)) reacting with iohexol and diatrizoate in UV/PS process. Experimental conditions: UV intensity = 0.93 mW/cm^2, $[\text{iohexol}]_0 = [\text{diatrizoate}]_0 = [\text{BA}]_0 = 10\ \mu\text{M}$, $[\text{PS}]_0 = [\text{H}_2\text{O}_2]_0 = 200\ \mu\text{M}$, $[\text{phosphate buffer}]_0 = 10\ \text{mM}$, Temp. = 25 ± 1 °C, and pH = 7.
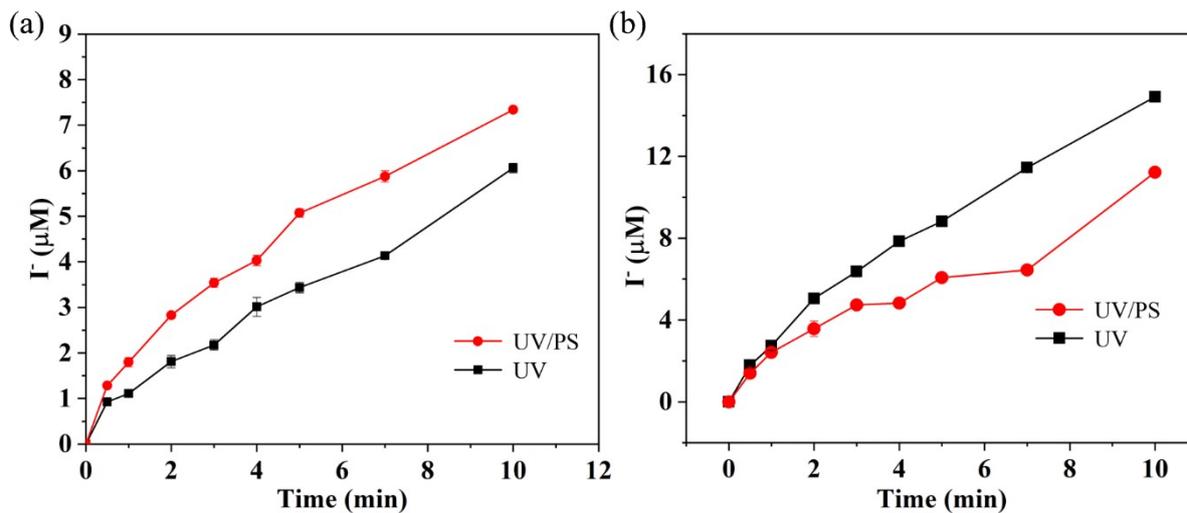
Figure S3 I⁻ production of (a) iohexol and (b) diatrizoate in UV alone and UV/PS processes.

Experimental conditions: UV intensity = 0.93 mW/cm², [iohexol]$_0$ = [diatrizoate]$_0$ = 10 μM,

[PS]$_0$ = 200 μM, [phosphate buffer]$_0$ = 10 mM, Temp. = 25 ± 1 °C, and pH = 7.
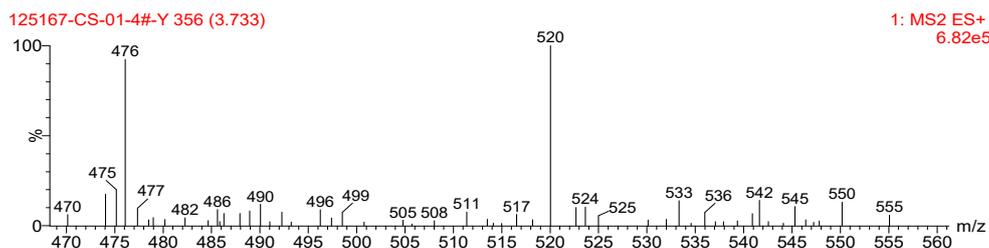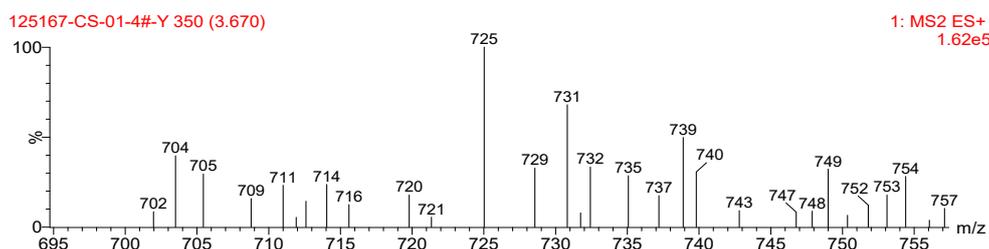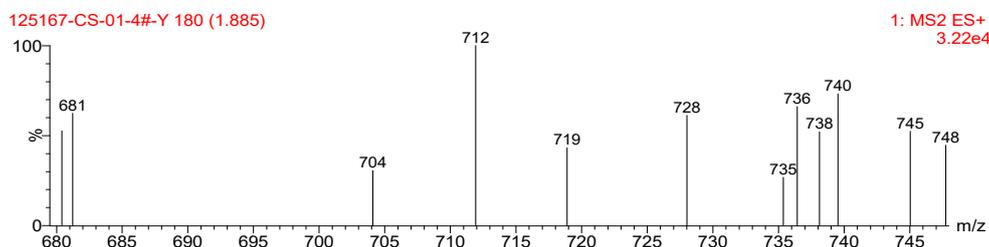
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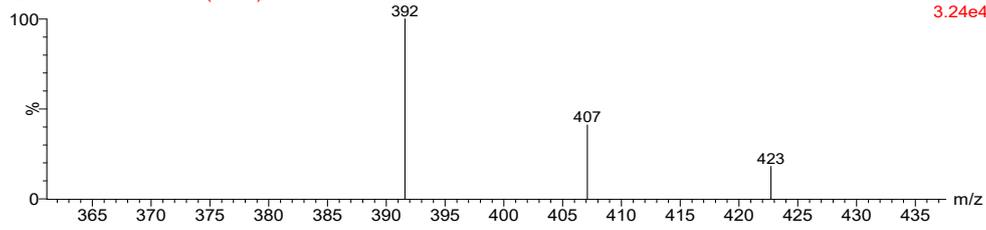
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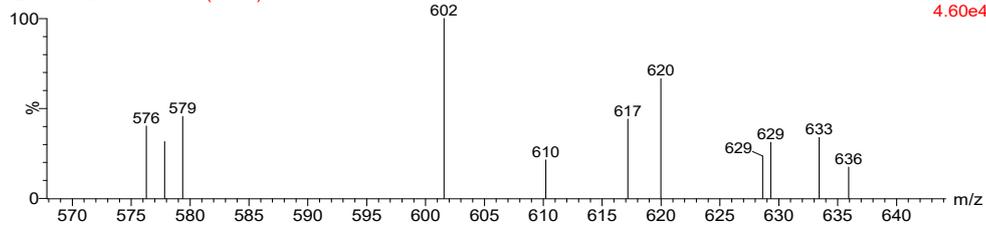
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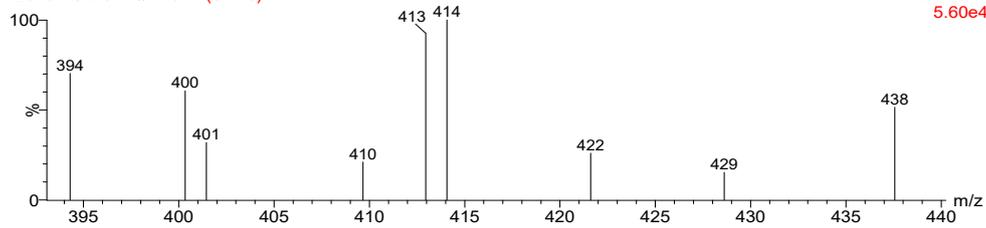
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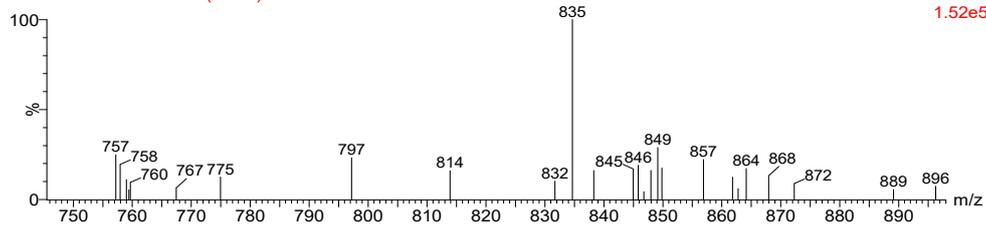
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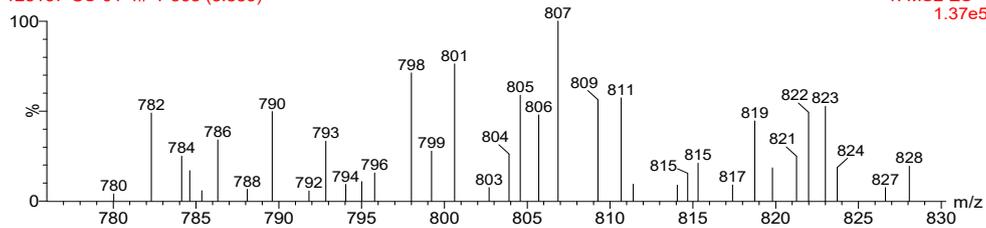
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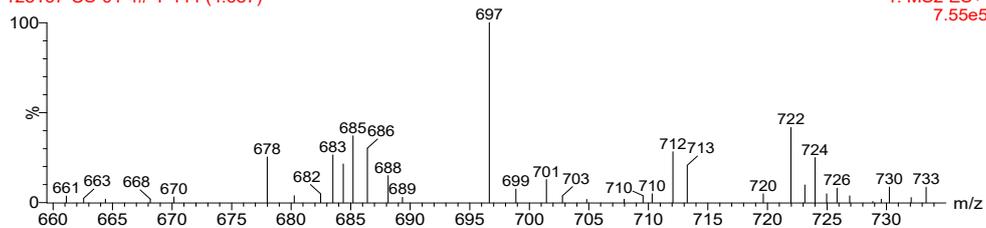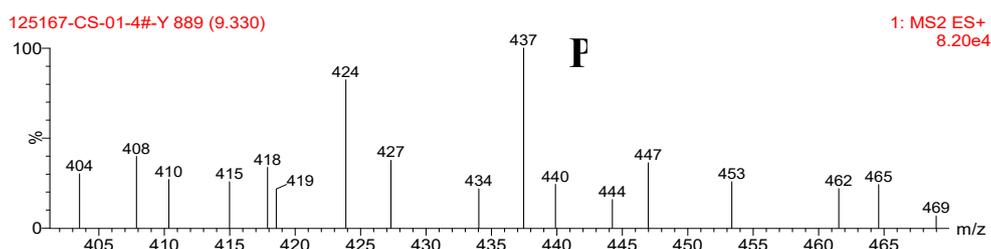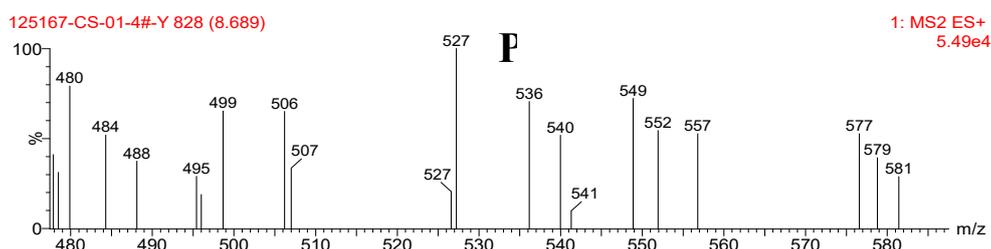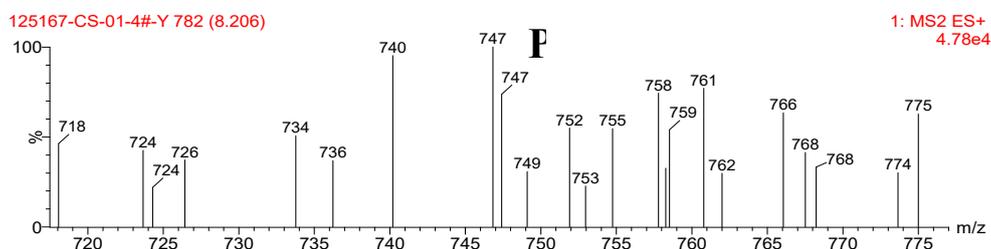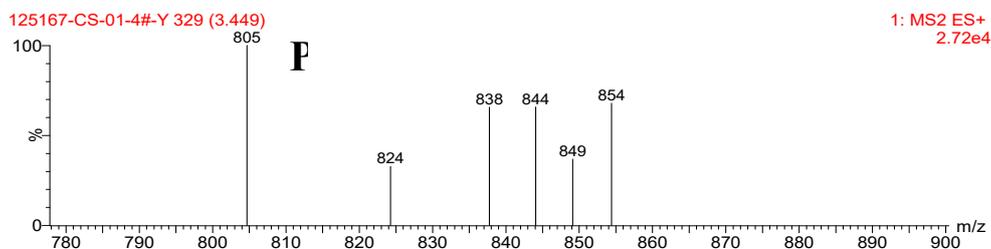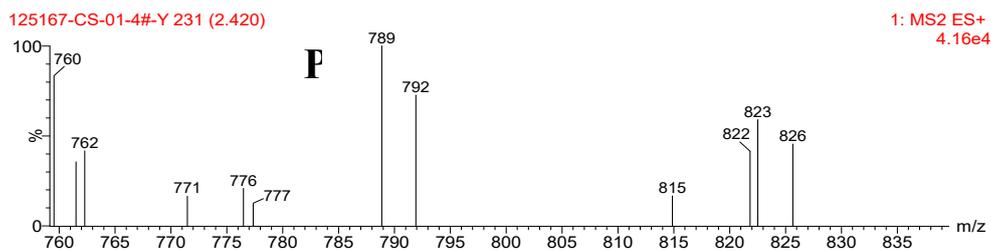
Figure S4 Mass spectra of the degradation of iohexol by UV/PS process.

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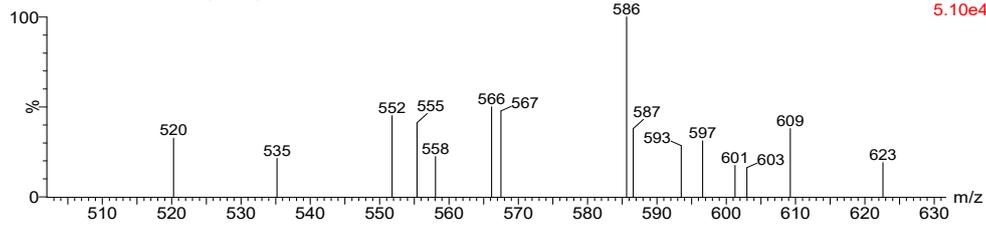
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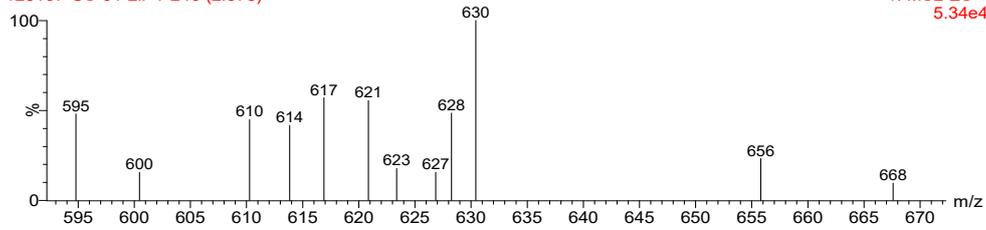
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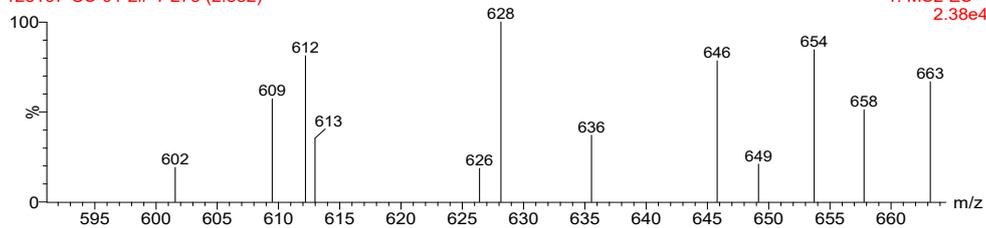
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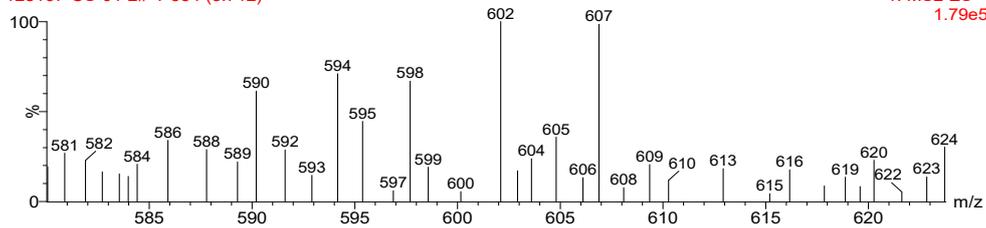
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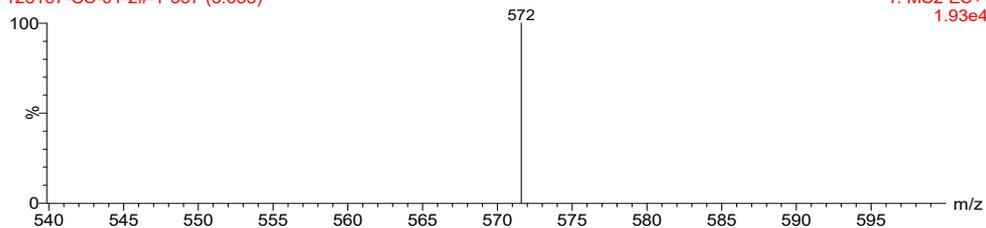
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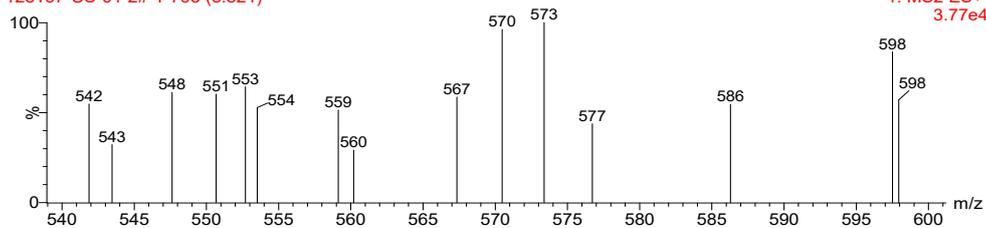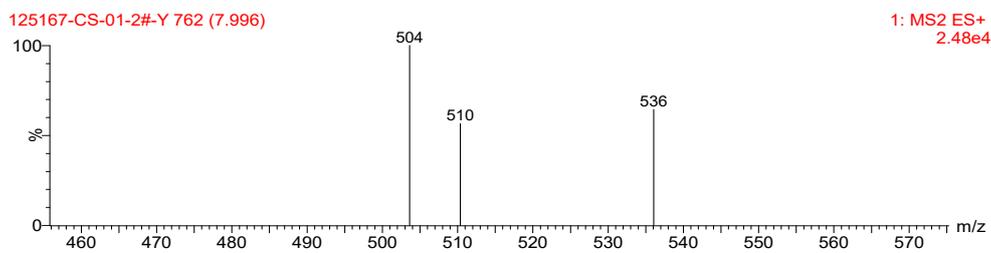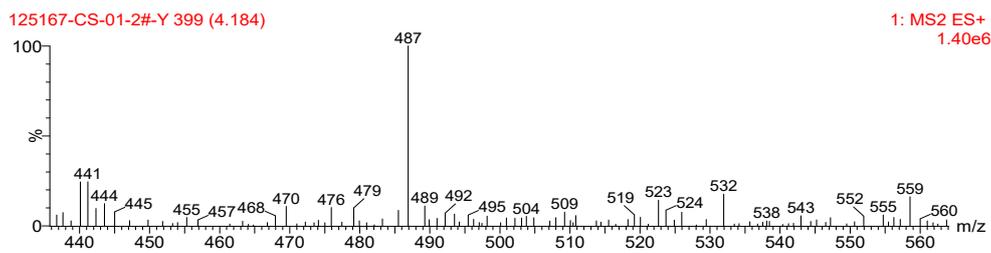
**Figure S5** Mass spectra of the degradation of diatrizoate by UV/PS process.

Table S1 The detected intermediates during the degradation of iohexol by UV/PS process.

| Number	m/z	Proposed structure	Number	m/z	Proposed structure
P1	711		P8	807	
P2	725		P9	697	
P3	519		P10	789	
P4	393		P11	805	
P5	602		P12	747	
P6	414		P13	527	
P7	835		P14	437	
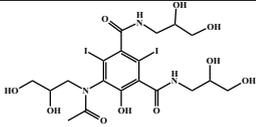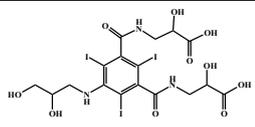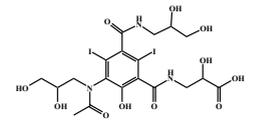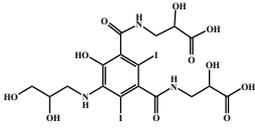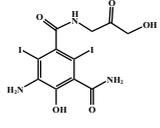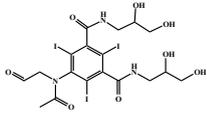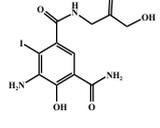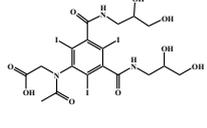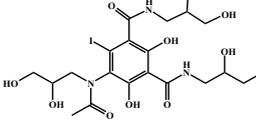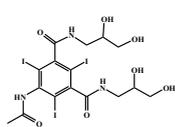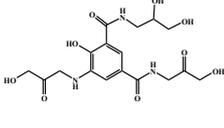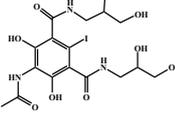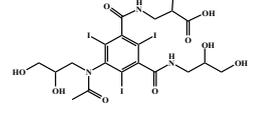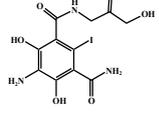
Table S2. The detected intermediates during the degradation of diatrizoate by UV/PS process.

Number	m/z	Proposed structure
P1	586	
P2	630	
P3	628	
P4	602	
P5	572	
P6	573	
P7	486	
P8	504	
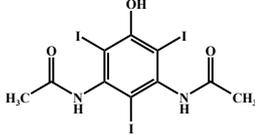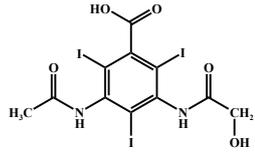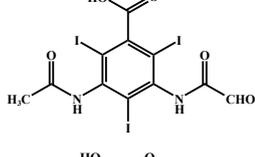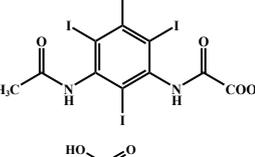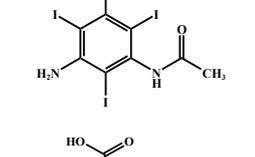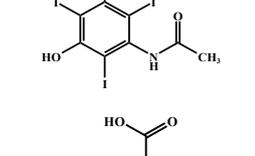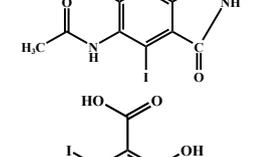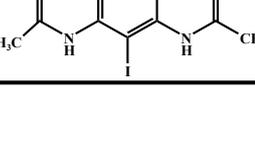
References

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https://doi.org/https://doi.org/10.1016/j.jphotochem.2021.113482