Supplementary Information for:

Impact of nitrite on the formation of trichloronitromethane during the UV-LED/chlorine process

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List of supporting information

Text S1. Chemicals.

Bisphenol A, HPLC-grade methanol and formic acid, analytical standard THMs, and trichloronitromethane (TCNM) were obtained from Sigma-Aldrich (MO, USA). Ascorbic acid, sodium thiosulfate (NaS_2O_3), NaH_2PO_4, Na_2HPO_4, $NaNO_2$, sodium hypochlorite (NaOCl) were purchased from Sinopharm (Shanghai, China). All solutions were prepared with ultrapure water (18.2 MΩ cm) produced by a Milli-Q water purification system (Millipore, Reference).

Text S2. Methods of Purge-and-trap and GC-MS to determine THMs and TCNM.

The formed THMs and HANs were detected by purge-and-trap gas chromatography–mass spectrometry (PT-GC-MS). The purge-and-trap sample concentrator (Tekmar Lumin, USA) used as a pretreatment can enrich volatile DBPs, which is then coupled to GC-MS (7890A-5975C, Agilent, USA) analysis. The instrumentation details are as follows: (1) purge and trap analysis: 5 mL of sample was injected into the U-tube chamber and purged at 20 ℃ for 11 min with helium at 40 mL min^{-1}; followed by the desorb mode, the trap was risen to 250 ℃ for 2 min at the flow rate of 300 mL min^{-1}; and finally baked at 280 ℃ for 2 min to clean up the trap. (2) GC–MS analysis: the initial temperature of the oven began at 30 ℃ for 9 min, increased to 40 ℃ at 2 ℃ min-1 and maintained for 1 min, and then raised up to 80 ℃ at 20 ℃ min^{-1}, then raised up to 160 ℃ at 40 ℃ min^{-1} and maintained for 2 min, and finally reached up to 250 ℃ at 50 ℃ and maintained for 1 min; with a split ratio of 10:1.

Text S3. Methods for calculating theoretical cytotoxicity and genotoxicity of DBPs (THMs and TCNM).

The cytotoxicity and genotoxicity of formed DBPs was calculated by eqs. S1-2.

$$\text{Cytotoxicity of DBPs} = \frac{\text{Concentration of DBP}}{LC_{50}\ \text{of DBP}} \quad \text{* MERGEFORMAT (S1)}$$

$$\text{Genotoxicity of DBPs} = \frac{\text{Concentration of DBP}}{\text{SCGE Genotoxic Potency of DBP}} \quad \text{(S2)}$$

CHO cells are widely used in toxicology. The $LC5_0$ value is the concentration of each individual DBP inducing a 50% reduction in the density of Chinese Hamster Ovary cells for 72h[1]. The LC_{50} values of individual DBPs were available in the literature[2]. This approach has been used to assess toxicity of measured DBPs and evaluate the contribution of individual DBPs to the total DBP-associated toxicity[3].

Table S1. Chinese hamster ovary cell cytotoxicity and genotoxicity of DBPs identified in this study.

DBPs	LC_{50} (M)	SCGE Genotoxic Potency (M)	Reference
TCM	9.62×10^{-3}	1×10^{-2}	4, 5
TCNM	5.36×10^{-4}	9.34×10^{-5}	5

*LC_{50} and SCGE Genotoxic Potency of DBPs means the concentration of DBP inducing a 50% reduction in the density of Chinese Hamster Ovary cells for 72h.

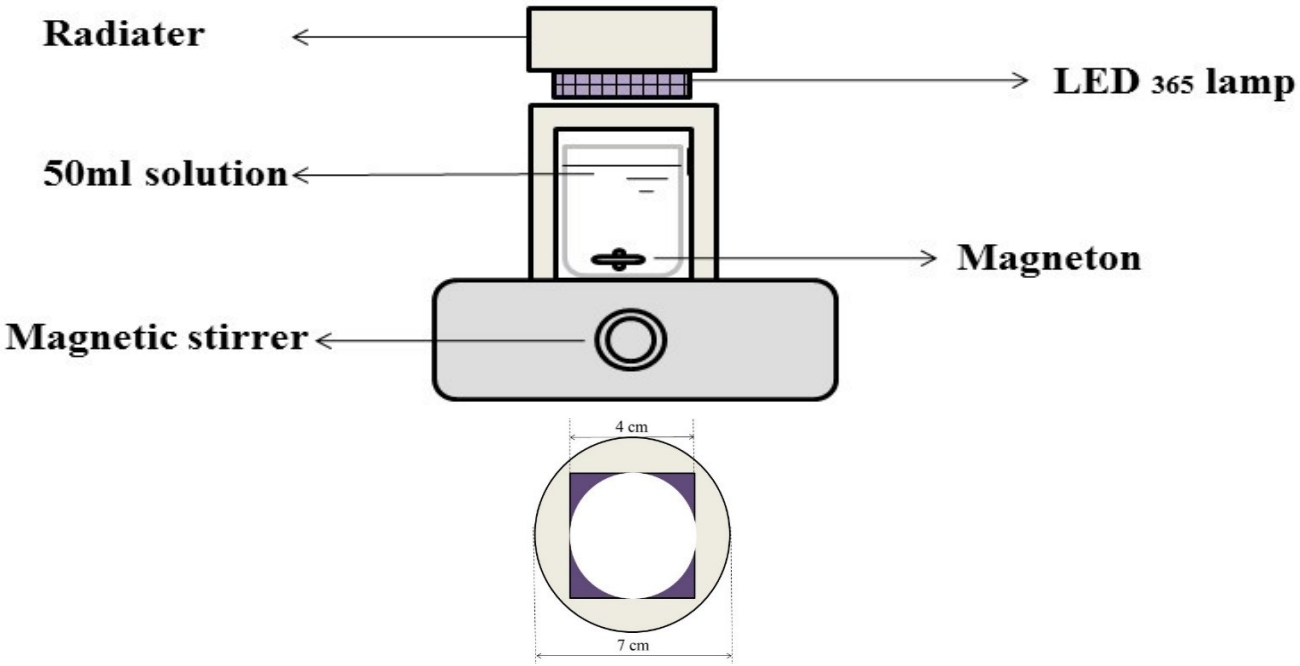

Figure S1. Schematic diagram of UV-LED (365 nm) reactors.

References

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