Supporting Information

for

Comparison of iodinated disinfection by-product formation from the reaction of chlorine, monochloramine, and organic chloramine with seaweed salt during the simulated household cooking process

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Text S1. Analytical methods.

10 mL aliquots of the sample were quenched with ascorbic acid at the same initial disinfectant molar concentration and extracted with 2 mL of methyl tert-butyl ether (MtBE). Then, the solution was shaken by a multi-tube vortex mixer (DMT-2500, Shanghai, China) at 2300 rpm for 5 min, and the samples were settled down for 5 min. Finally, 1 mL of the organic phase was withdrawn and analyzed by Shimadzu QP2010plus gas chromatography equipped with electron capture detection (GC/ECD, Kyoto, Japan). The column was a Restek RTX-5MS silica capillary one (30 m × 0.25 mm, I.D. with 0.25 μm film thickness, Bellefonte, USA). The injector temperature and detector temperature were 200 ℃ and 280 ℃, respectively. The oven program was holding at 35 ℃ for 10 min, then ramping to 200 ℃ at 20 ℃/min and holding for 5 min.

Text S2. The sample pretreatment for toxicity determination

Sulfuric acid was added into 500 mL of each sample to acidify to pH <0.5 and saturated with sodium sulfate. Then the water sample was extracted with 50 mL MtBE three times. The organic phase was concentrated to approximately 5 mL by rotary evaporator and evaporated all MtBE by nitrogen gas. The remaining solid was stored at -18 ℃. The solid was dissolved by Dulbecco's modified Eagles medium (DMEM) (containing 0.5% of dimethyl sulfoxide (DMSO)) to prepare a stock solution before use. And the stock solution was diluted into different concentrations to test cytotoxicity. Mean cell concentration values were calculated as a percentage of the mean negative control value (set at 100% viability).

Table S1. Characteristics of seaweed salts [1].

Parameters	Salt-1	Salt-2
I^- (mg I/g)	0.025 ± 0.002	0.029 ± 0.003
DOC (mg/g)	0.072 ± 0.002	0.019 ± 0.001
UV_{254}*	0.060 ± 0.001	0.050 ± 0.001
TOI (mg I/g)	0.023 ± 0.001	0.012 ± 0.001

* The value represents the absorbance at 254 nm of salt solution (10 g/L).

Table S2. Characteristics of water samples.

Parameters	Tap water A	Tap water B	Tap water C
DOC (mg/L)	1.51 ± 0.3	2.10	2.13
Total chlorine (mg/L)	⩽0.02	1.02	0.93
Free chlorine (mg/L)	-	0.88	0.07
Monochloramine (mg/L)	-	0.00	0.84
Other reactive chlorine species (mg/L)	-	0.14	0.02

Table S3. Characteristics, sources, and limit of quantitation of the DBP.

DBPs	CAS No.	Chemical formula	Molecular weight	LC_{50} (M) [2]	Limit of detection (μg/L)	Limit of quantitation (μg/L)	Source and purity
TCM	67-66-3	$CHCl_3$	119.38	9.62×10^{-3}	0.19	0.63	Supelco, 99%
BDCM	75-27-4	$CHBrCl_2$	163.83	1.15×10^{-2}	0.12	0.39	Supelco, 99%
DBCM	124-48-1	$CHBr_2Cl$	208.28	5.36×10^{-3}	0.19	0.63	Supelco, 99%
TBM	75-25-2	$CHBr_3$	252.73	4.13×10^{-3}	0.82	2.72	Supelco, 99%
DCIM	594-04-7	$CHCl_2I$	210.83	3.96×10^{-3}	0.19	0.64	CanSyn, >95%
CDIM	638-73-3	$CHClI_2$	302.28	1.91×10^{-3}	0.56	1.87	CanSyn, 90-95%
DBIM	593-94-2	$CHBr_2I$	299.73	2.41×10^{-3}	0.26	0.86	CanSyn, 90-95%
BDIM	557-95-9	$CHBrI_2$	346.73	1.40×10^{-3}	0.21	0.69	CanSyn, 90-95%
TIM	75-47-8	CHI_3	393.73	6.60×10^{-5}	0.20	0.67	Aladdin, 99%

Table S4. Henry's law constant of disinfectants [3].

Disinfectant	Henry's law constant (atm-m^3/M)
Organic chloramine (N-Chloroglycine)	2.56×10^{-7}
HOCl	3.22×10^{-5}
NH_2Cl	3.37×10^{-4}

Table S5. One-way ANOVA results.

Water Sample	Variance	Quadratic sum	Degree of freedom	Mean square	F	Statistical significance*
Heated Tap water B	Between groups	0.50	8	0.06	1.197	**0.354**
	Within groups	0.94	18	0.05		
	Total statistic data	1.44	26			
Heated Tap water B with Salt-1	Between groups	0.785	8	0.098	24.799	**< 0.001** *
	Within groups	0.071	18	0.004		
	Total statistic data	0.856	26			
Heated Tap water C	Between groups	0.612	8	0.077	1.226	**0.340**
	Within groups	1.124	18	0.062		
	Total statistic data	1.736	26			
Heated Tap water C with Salt-1	Between groups	0.182	8	0.023	1.469	**0.236**
	Within groups	0.278	18	0.015		
	Total statistic data	0.460	26			

*Statistical significance < 0.05 was regarded as significant variation by concentration factor.

Figure S1. Disinfectant concentration variation at different temperatures in ultrapure water.

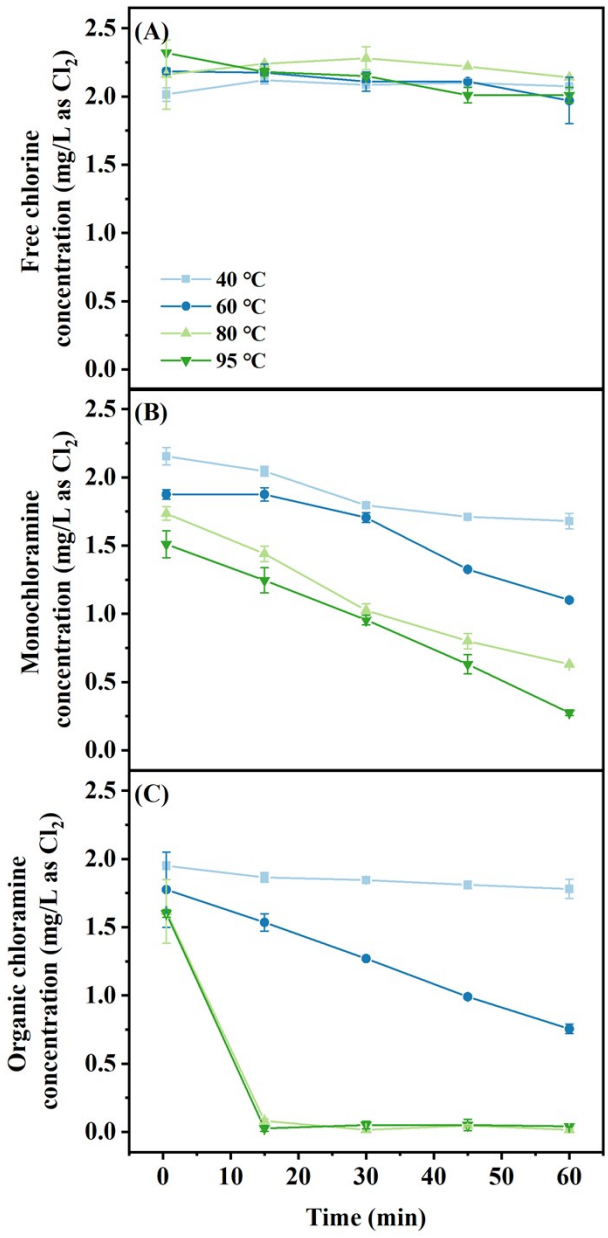


Figure S2. Fluorescence EEM spectra with chlorination (C and I), chloramination (D and J), performed organic chloramination (E and K) and in situ organic chloramination (F and L) or without disinfectant (B and H) during simulated household cooking with Tap water A (Reaction condition: seaweed iodine table salt dose = 10.0 g/L, disinfectant dose = 2.0 mg/L, temperature = 80 °C, time = 1.0 h, and unbuffered). A and G were UP water and reacted at the same condition. A~F were added Salt-1, while G~L were added Salt-2.

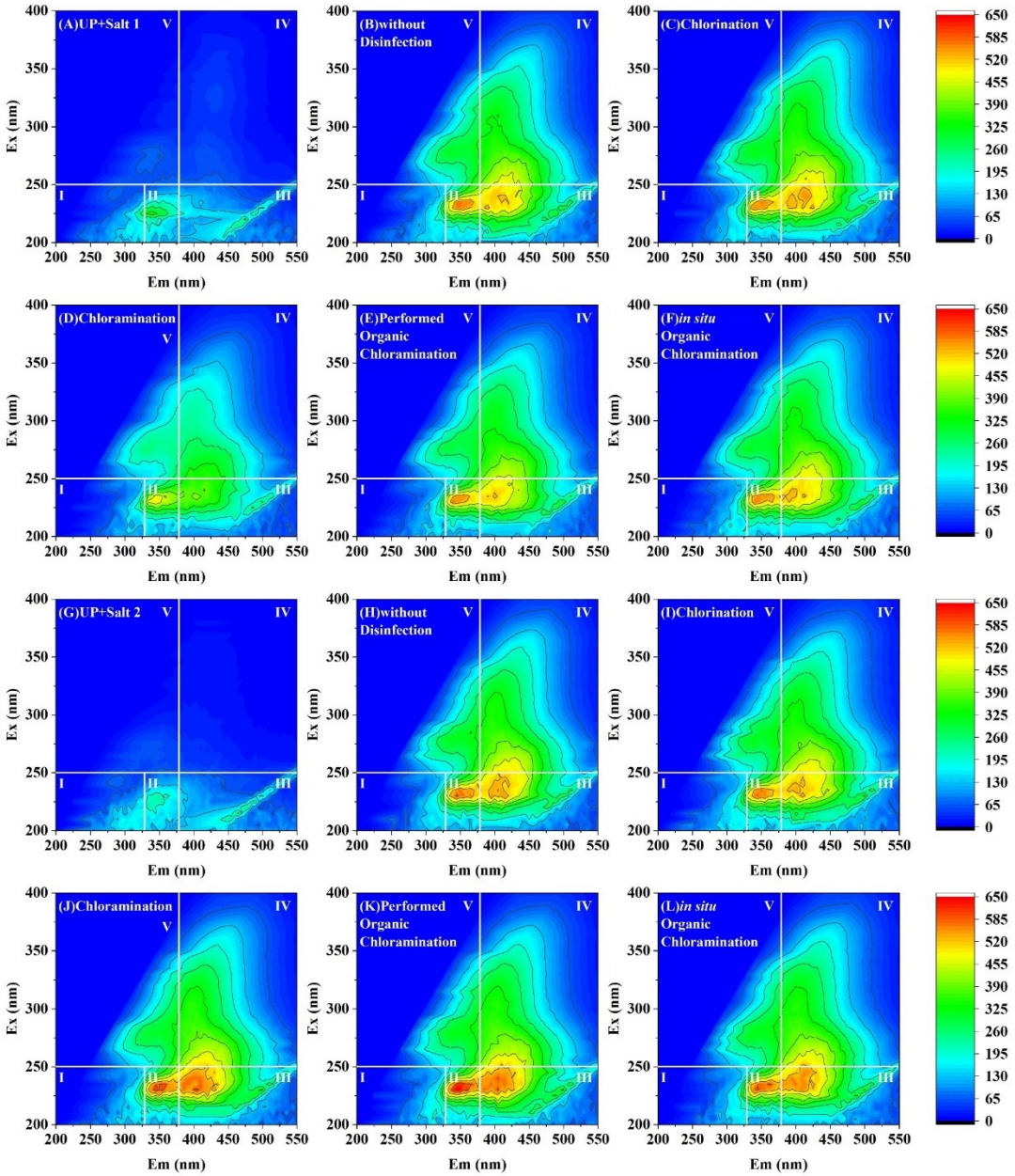
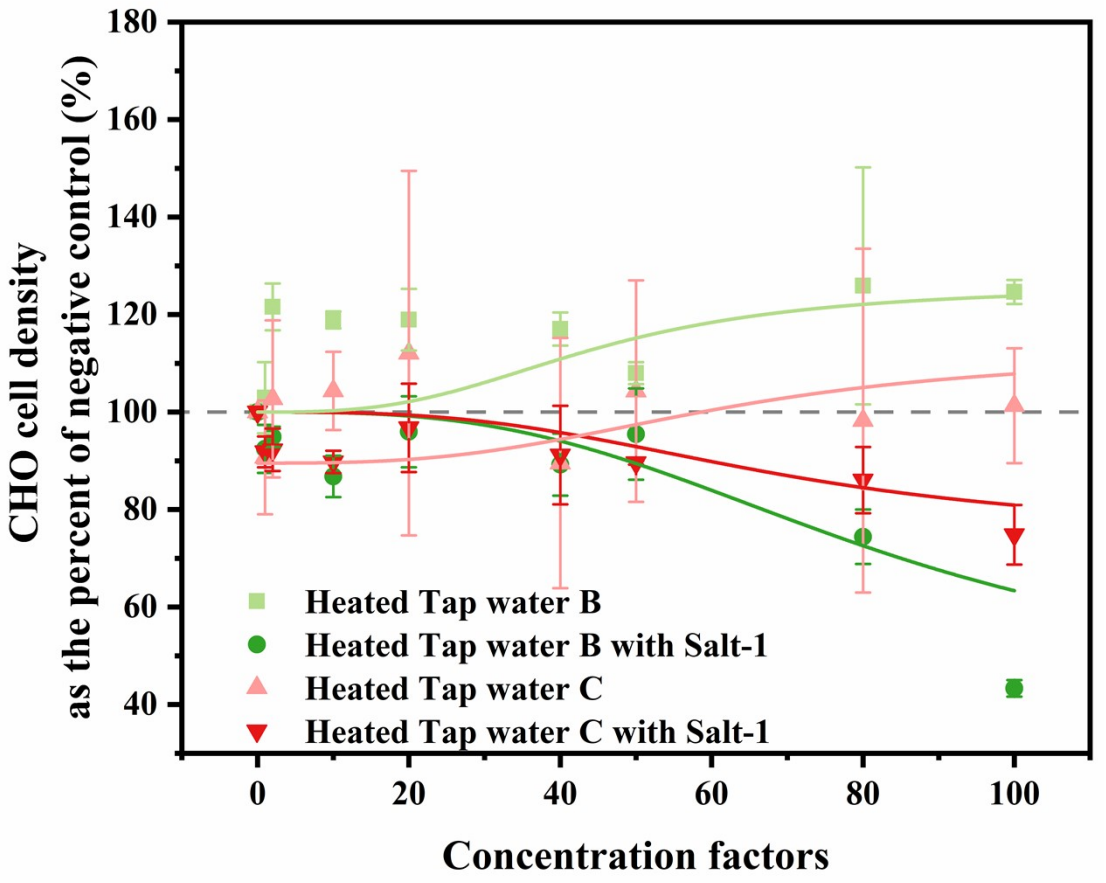


Figure S3. CHO cell chronic cytotoxicity of DBP mixture in Tap water B and Tap water C during simulated household cooking with seaweed iodine table salt. (Salt dose = 10.0 g/L, temperature = 80 ℃, reaction time=1 h.)



References

1. Z. Cao, S. Ding, Y. Deng, X. Luan and W. Chu, Household cooking with seaweed salts and chloraminated tap water produce harmful iodinated disinfection by-products, *Chem Eng J*, 2022, **431**, 133471.
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3. S. J. Judd and S. H. Black, Disinfection by-product formation in swimming pool waters: A simple mass balance, *Water Res*, 2000, **34**, 1611-1619.