

Electronic Supplementary Information for
Occurrence, Profiling and Prioritization of Halogenated Disinfection By-Products in
Drinking Water of China

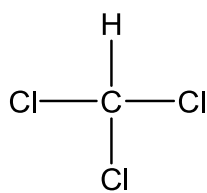
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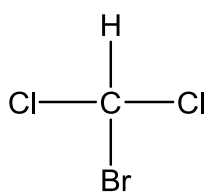
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China

Figure 1

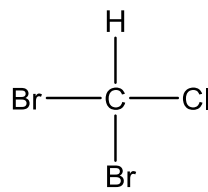
Tables 8



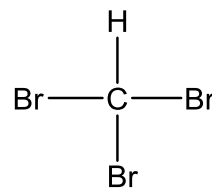
TCM



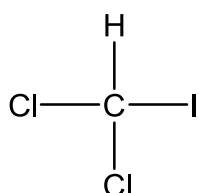
DCBM



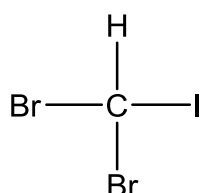
DBCM



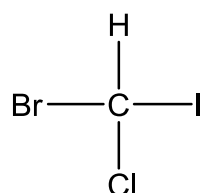
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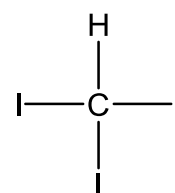
DCIM



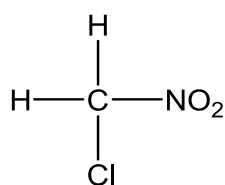
DBIM



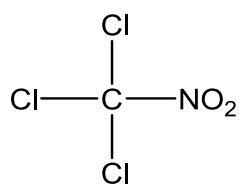
BCIM



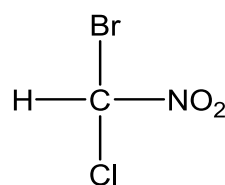
TIM



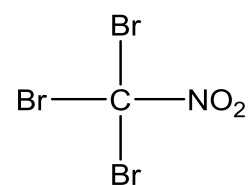
CNM



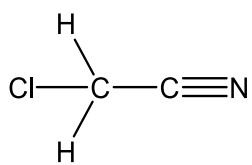
TCNM



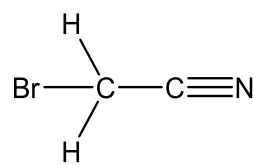
BCNM



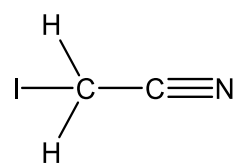
TBNM



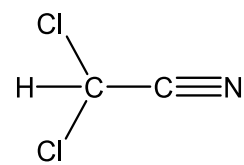
CAN



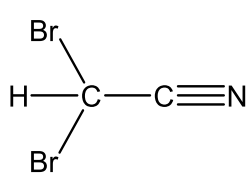
BAN



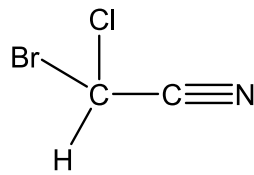
IAN



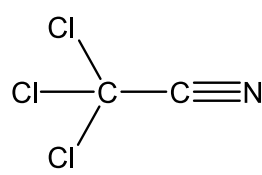
DCAN



DBAN



BCAN



TCAN

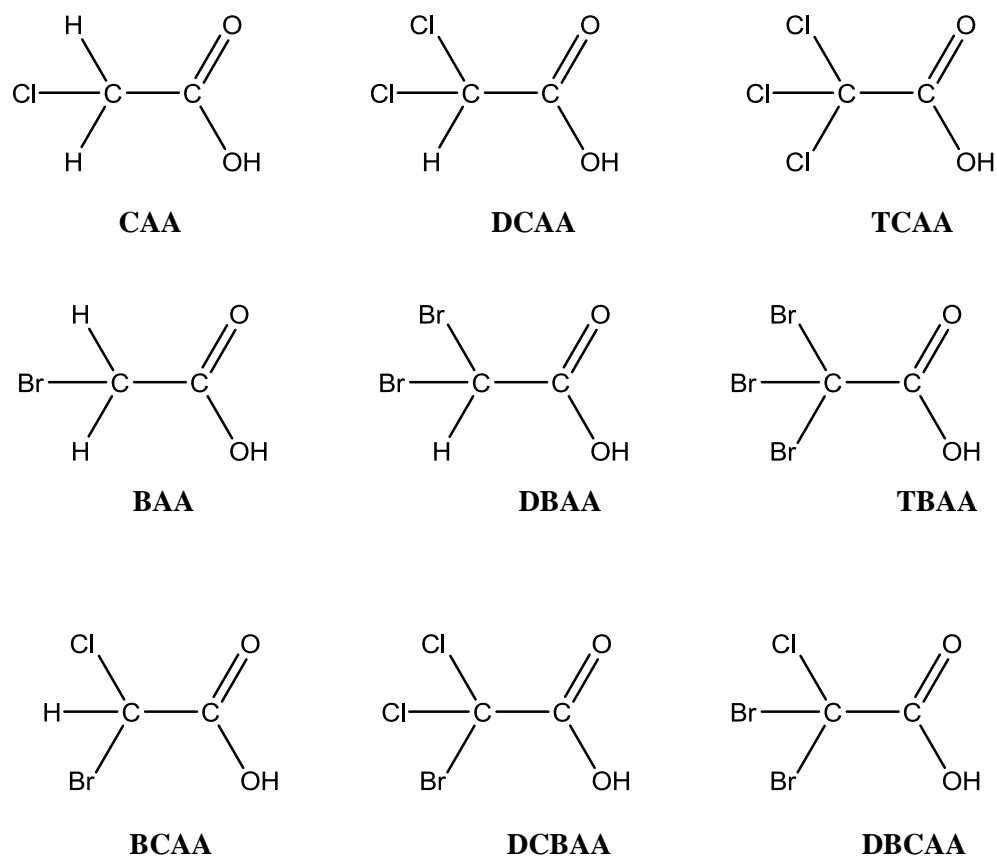


Figure S1. The structures and acronyms of target analytes.

Table S1. Limit of quantization (LOQs, $\mu\text{g L}^{-1}$) and recoveries (n=3) of DBPs in drinking waters.

	Cmpound	Acronym	LOQs ($\mu\text{g L}^{-1}$)	Recoveries (mean \pm RSD)
THM4	Chloroform	TCM	0.2	105 \pm 17.4
	Bromodichloromethane	BDCM	0.01	113 \pm 8.0
	Dibromochloromethane	DBCM	0.03	102 \pm 13.2
	Bromofrom	TBM	0.05	130 \pm 12.7
Iodinated THMs	Dichloriodomethane	DCIM	0.1	111 \pm 10.7
	Bromochloriodomethane	BCIM	0.1	114 \pm 8.6
	Dibromiodomethane	DBIM	0.1	102 \pm 11
	Iodoform	TIM	0.1	91 \pm 7.0
HAAs	Monochloroacetic acid	CAA	2.08	80.8 \pm 1.5
	Dichloroacetic acid	DCAA	0.45	97.0 \pm 6.4
	Trichloroacetic acid	TCAA	1.09	101 \pm 0.5
	Monobromoacetic acid	BAA	0.70	80.1 \pm 1.1
	Dibromoacetic acid	DBAA	1.25	98.0 \pm 3.9
	Tribromoacetic acid	TBAA	24.29	88.8 \pm 0.6
	Bromochloroacetic acid	BCAA	0.56	101 \pm 2.7
	Bromodichloroacetic acid	BDCAA	3.10	98.3 \pm 4.4
	Chlorodibromoacetic acid	CDBAA	4.00	93.5 \pm 13
HANs	Chloroacetonitrile	CAN	0.02	71 \pm 6.7
	Dichloroacetonitrile	DCAN	0.02	97 \pm 7.5
	Trichloroacetonitrile	TCAN	0.01	97 \pm 4.4
	Bromoacetonitrile	BAN	0.01	82 \pm 12.8

HNM s	Dibromoacetonitrile	DBAN	0.05	122 ± 15
	Bromochloroacetonitrile	BCAN	0.01	110 ± 7.5
	Iodoacetonitrile	IAN	0.2	87 ± 7.8
	Chloronitromethane	CNM	0.01	92 ± 4.9
	Trichloronitromethane	TCNM	0.01	85 ± 3.5
	Bromochloronitromethane	BCNM	0.1	94 ± 6.3
	Tribromonitromethane	TBNM	0.3	98 ± 6.2
Internal standars	Bromofluorobenzene			99 ± 3.7
	1,2-dibromopropane			105 ± 2.2
	decafluorobiphenyl			113 ± 11.6

Table S2 Optimized instrumental and SRM conditions of HAAs.

Retention time (min)	compound	Dwell time (s)	Precursor ion	Product ion	Cone Voltage (V)	Collision energy (eV)
1.42	CAA	0.07	92.6	34.8	20	11
1.58	BAA	0.05	136.7	78.5	20	10
1.69	DCAA	0.05	126.6	82.6	20	10
1.81	BCAA	0.05	172.7	128.7	20	9
1.96	DBAA	0.05	216.8	172.8	20	11
2.89	TCAA	0.05	160.6	116.6	15	8
3.03	BDCAA	0.05	206.8	162.6	16	7
3.15	CDBAA	0.10	250.8	206.7	15	7
3.31	TBAA	0.08	249.0	78.5	30	20

Table S3. DBPs measured in drinking water samples collected from 70 water treatment plants ($\mu\text{g L}^{-1}$) and major water quality parameters.

DBP	1 ^a	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
TCM	5.34	5.27	13.48	0.21	9.13	6.59	6.03	5.41	5.93	5.07	5.72	7.29	6.22	6.45	5.99	12.17	3.52	5.90
BDCM	1.28	2.75	3.85	0.36	1.84	0.12	0.74	0.77	0.99	1.00	0.17	3.45	0.79	0.63	1.07	0.73	0.66	1.79
DBCM	ND ^b	0.50	0.77	0.22	0.18	0.04	0.44	0.08	0.33	0.91	0.08	0.91	0.12	0.14	0.24	0.49	0.19	0.50
TBM	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.16	ND	ND	ND	ND	0.12	ND	ND	ND
THM4	6.62	8.52	18.10	0.79	11.15	6.75	7.21	6.27	7.25	7.14	5.97	11.65	7.12	7.22	7.41	13.39	4.37	8.19
DCIM	ND	ND	ND	ND	ND	ND	ND	ND	0.46	ND	ND	0.26	0.53	0.48	ND	ND	ND	0.71
BCIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
DBIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
TIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
I-THMs	ND	ND	ND	ND	ND	ND	ND	ND	0.46	ND	ND	0.26	0.53	0.48	ND	ND	ND	0.71
CAA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
DCAA	6.69	ND	6.93	4.57	4.41	3.92	0.95	2.99	13.86	4.63	1.11	4.09	ND	2.68	4.12	5.21	3.85	12.59

IAN	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
HANs	0.30	0.69	0.07	0.14	0.54	0.28	0.17	0.16	0.95	0.17	0.15	1.15	0.34	0.28	0.19	0.38	0.58	1.07	
CNM	ND	0.12	0.15	0.05	0.04	0.02	0.03	0.04	0.04	0.04	0.03	0.04	0.03	0.03	0.05	0.04	ND	0.07	
TCNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
BCNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
TBNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
HNM_s	ND	0.12	0.15	0.05	0.04	0.02	0.03	0.04	0.04	0.04	0.03	0.04	0.03	0.03	0.05	0.04	ND	0.07	
TOC (mg L ⁻¹)	5.45	3.82	- ^c	-	2.20	-	1.64		2.97	1.06	2.49	1.63	2.47	2.28	-	-	1.61	2.41	
Br ⁻ (µg L ⁻¹)	2.95	-	-	-	9.01		19.08		11.02	34.60		19.38	10.04	7.58			10.53	23.53	
I ⁻ (µg L ⁻¹)	ND	-	-	-	ND		ND		ND	ND		ND	ND	ND			ND	ND	
NH ₄ ⁺ (mg L ⁻¹)	<0.01	0.18	-	-	0.19	0.13	0.82	<0.02	0.02	-	-	-	0.97	0.50	0.26	-	-	0.53	
disinfectant	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	NH ₂ Cl	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	NH ₂ Cl	NH ₂ Cl	Cl ₂	ClO ₂	Cl ₂	NH ₂ Cl	
SW ^f type	river	river	river	river	river	river	river	river	LR ^d	GW ^e	LR	LR	LR	LR	river	river	river	river	

DBP	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
TCM	6.56	4.92	4.42	4.36	6.55	7.04	9.59	6.96	7.03	8.49	5.80	8.95	4.08	0.89	7.42	8.75	5.83	10.31
BDCM	1.15	0.12	0.88	1.34	1.53	0.60	0.97	0.46	0.44	0.07	0.55	0.69	1.42	1.32	2.55	1.93	2.45	6.30
DBCM	0.61	0.40	0.43	1.10	0.52	0.50	0.40	0.23	0.17	0.03	0.18	0.26	1.06	0.73	7.76	3.35	0.98	2.12
TBM	0.41	0.09	0.43	0.19	ND	ND	ND	ND	ND	ND	ND	ND	0.33	0.39	3.82	0.97	0.78	0.88
THM4	8.72	5.53	6.16	6.99	8.60	8.14	10.96	7.65	7.63	8.59	6.53	9.90	6.89	3.33	21.56	14.99	10.03	19.62
DCIM	ND	ND	1.30	0.44	1.27	1.24	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
BCIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
DBIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
TIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
I-THMs	ND	ND	1.30	0.44	1.27	1.24	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
CAA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
DCAA	1.15	9.66	8.82	3.78	10.04	52.85	9.66	3.66	6.66	10.91	8.33	8.11	3.95	1.38	2.95	3.71	3.58	3.45
TCAA	2.55	ND	6.79	2.23	10.12	6.79	5.14	3.18	4.46	7.11	11.19	12.12	1.65	1.12	2.49	4.59	3.94	2.55

HANs	0.86	0.65	1.94	0.76	1.31	0.77	6.08	4.37	1.56	1.13	0.20	2.66	0.97	1.38	1.07	1.75	ND	4.60	
CNM	ND	ND	0.06	0.02	0.07	0.01	0.06	ND	0.07	ND	0.11	0.07	0.03	0.11	0.05	0.09	0.96	0.05	
TCNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
BCNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
TBNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
HNM_s	ND	ND	0.06	0.02	0.07	0.01	0.06	ND	0.07	ND	0.11	0.07	0.03	0.11	0.05	0.09	0.96	0.05	
TOC (mg L ⁻¹)	1.70	2.19	2.16	2.28	2.17	2.23	2.02	2.67	-	2.11	1.98	-	3.10	5.30	2.53	2.38	2.28	2.28	
Br ⁻ (µg L ⁻¹)	30.29	28.12	9.83	-	22.76	13.39	14.53	10.38	-	3.88	16.40	-	ND	242.50	139.88	103.46	26.95	23.77	
I ⁻ (µg L ⁻¹)	ND	ND	ND	-	ND	ND	ND	ND	-	ND	ND	-	ND	ND	ND	ND	ND	ND	
NH ₄ ⁺ (mg L ⁻¹)	0.05	0.07	-	-	-	-	-	-	-	<0.04	<0.04	<0.04	-	0.08	0.08	1.20	0.14	0.25	
disinfectant	Cl ₂	ClO ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	NH ₂ Cl	Cl ₂	Cl ₂
SW type	river	LR	LR	LR	LR	LR	river	river	river	LR	river	river	river	river	river	river	LR	river	river

DBP	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
TCM	5.67	15.39	12.45	5.52	5.45	15.98	21.34	24.60	10.37	5.89	5.47	2.80	0.61	3.66	1.59	3.94	11.30	13.60
BDCM	2.90	2.11	3.37	0.87	0.17	5.50	9.14	7.76	15.35	8.72	10.28	7.73	1.52	7.71	1.37	17.02	2.13	4.58
DBCM	0.99	0.35	0.49	ND	0.10	0.62	2.49	1.20	13.41	6.40	5.95	5.90	2.41	10.76	2.33	18.80	0.24	ND
TBM	0.53	0.41	0.30	ND	ND	3.46	9.14	73.47	3.76	0.97	0.91	ND	5.31	5.19	1.58	6.97	26.91	ND
THM4	10.10	18.26	16.62	6.39	5.73	25.58	42.11	107.03	42.89	21.98	22.61	16.42	9.85	27.32	6.87	46.73	40.58	18.18
DCIM	ND	ND	ND	ND	ND	0.62	1.01	1.20	1.37	ND	0.74	0.51	ND	1.94	ND	3.67	ND	ND
BCIM	ND	ND	ND	ND	ND	0.68	ND	1.75	ND	ND	ND	ND	ND	ND	ND	1.91	ND	ND
DBIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
TIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
I-THMs	ND	ND	ND	ND	ND	1.31	1.01	2.95	1.37	ND	0.74	0.51	ND	1.94	ND	5.58	ND	ND
CAA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
DCAA	2.01	ND	6.05	2.00	2.76	3.44	3.90	3.64	4.90	4.82	10.64	6.71	3.51	1.53	ND	3.80	20.13	16.76
TCAA	2.35	9.84	7.25	ND	ND	7.59	6.96	7.01	6.27	2.89	5.91	5.31	4.16	ND	ND	ND	4.91	5.36

BAA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
BCAA	ND	ND	1.96	2.24	ND	ND	2.57	ND	ND	2.32	3.15	3.82	2.35	1.53	1.83	3.03	ND	ND	
DBAA	ND	ND	ND	ND	ND	ND	ND	ND	ND	1.26	2.77	2.83	1.71	2.33	2.41	2.87	3.32	ND	ND
DCBAA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	3.13	ND	ND	ND	3.38	ND	ND
DBCBA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	4.83	ND	ND	ND	4.09	ND	ND
TBAA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
HAAs	4.36	9.84	15.27	4.24	2.76	11.03	13.43	10.65	12.43	12.80	22.53	25.51	12.35	5.47	4.70	17.62	25.05	22.12	
CAN	0.13	ND	0.05	ND	ND	ND	ND	ND	0.18	0.07	ND	ND	ND	ND	0.14	0.29	ND	ND	
DCAN	0.90	2.92	2.23	0.70	0.15	4.02	6.66	6.16	2.73	1.26	1.98	1.46	0.15	1.14	0.50	1.89	ND	0.06	
TCAN	ND	ND	ND	ND	ND	0.17	ND	0.36	0.25	ND	ND	ND	0.11	0.15	0.16	0.05	ND	0.97	
BAN	ND	ND	ND	ND	0.07	0.01	ND	0.06	ND	ND	ND	ND	ND	0.11	0.07	0.16	ND	0.07	
BCAN	ND	1.57	0.99	ND	ND	1.31	6.57	2.25	6.70	1.25	1.50	1.57	ND	3.61	ND	4.43	ND	ND	
DBAN	ND	ND	ND	ND	ND	ND	ND	ND	2.63	ND	ND	ND	ND	ND	ND	4.08	ND	ND	
IAN	ND	ND	ND	ND	ND	ND	ND	0.2	ND	ND	ND	ND	ND	ND	ND	0.86	ND	ND	

HANs	1.03	4.49	3.27	0.70	0.23	5.68	13.24	8.99	12.48	2.58	3.48	3.03	0.25	5.00	0.87	11.77	0.00	1.09
CNM	0.08	0.05	0.02	ND	0.06	ND	ND	ND	0.77	0.27	0.26	0.32	0.05	0.28	0.39	0.81	0.17	0.13
TCNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.28	0.11	ND	ND	ND	0.11	ND	ND
BCNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
TBNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
HNM s	0.08	0.05	0.02	ND	0.06	ND	ND	ND	0.77	0.27	0.54	0.42	0.05	0.28	0.39	0.92	0.17	0.13
TOC (mg L ⁻¹)	-	3.20	-	1.74	2.37	2.07	1.98	-	2.62	2.35	2.28	-	3.14	2.55	-	3.15	-	1.37
Br ⁻ (µg L ⁻¹)	-	42.85	-	18.57	10.36	12.21	27.30	-	ND	ND	ND	-	ND	ND	-	ND	-	17.10
I ⁻ (µg L ⁻¹)	-	ND	-	ND	ND	ND	ND	-	ND	ND	ND	-	ND	ND	-	ND	-	ND
NH ₄ ⁺ (mg L ⁻¹)	0.10	0.21	0.21	0.08	2.43	-	-	-	0.10	-	<0.02	0.61	0.34	0.05	0.18	0.14	0.20	0.23
disinfectant	Cl ₂	Cl ₂	Cl ₂	Cl ₂	NH ₂ Cl	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	NH ₂ Cl	Cl ₂	Cl ₂	ClO ₂	Cl ₂	Cl ₂
SW type	river	LR	LR	LR	river	river	river	river	river	river	LR	LR	LR	LR	LR	LR	river	river

DBP	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70
TCM	3.14	2.90	15.95	2.83	14.80	13.29	27.58	27.64	37.72	15.67	14.63	9.99	12.88	2.78	5.82	10.01
BDCM	6.10	1.16	31.00	0.52	7.13	10.75	10.09	16.03	11.40	1.98	27.81	19.32	21.25	3.67	7.73	9.66
DBCM	7.50	2.22	27.56	0.80	2.34	4.40	2.04	ND	2.47	0.20	21.41	17.87	19.11	6.08	9.68	5.17
TBM	1.77	1.01	5.52	0.40	ND	0.30	ND	0.31	0.63	ND	3.17	2.84	3.40	ND	2.91	0.89
THM4	18.51	7.28	80.03	4.56	24.27	28.74	39.71	43.98	52.22	17.85	67.03	50.02	56.65	12.54	26.15	25.73
DCIM	ND	ND	1.21	ND	ND	0.71	1.01	ND	2.00	ND	ND	ND	ND	ND	ND	0.60
BCIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
DBIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
TIM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
I-THMs	ND	ND	1.21	ND	ND	0.71	1.01	ND	2.00	ND	ND	ND	ND	ND	ND	0.60
CAA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
DCAA	2.84	2.20	3.89	6.86	5.48	3.59	9.44	4.88	15.62	7.71	0.00	7.31	7.93	0.45	2.11	ND
TCAA	1.29	ND	3.39	4.38	3.75	2.13	10.12	9.70	16.33	6.64	7.31	4.33	6.50	ND	1.59	1.25

HANs	0.51	0.79	5.48	0.76	3.98	2.95	14.66	22.84	4.46	6.91	27.50	39.20	18.36	2.32	21.53	2.64
CNM	0.07	0.06	0.18	ND	0.18	0.15	0.25	ND	0.02	ND	0.26	0.24	0.37	ND	0.07	0.03
TCNM	ND	ND	ND	ND	ND	0.07	ND	ND	ND	ND	ND	ND	ND	ND	0.02	ND
BCNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
TBNM	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
HNMs	0.07	0.06	0.18	ND	0.18	0.21	0.25	ND	0.02	ND	0.26	0.24	0.37	ND	0.09	0.03
TOC (mg L ⁻¹)	0.87	-	2.28	2.45	3.65	-	4.01	4.51	-	2.52	3.08	-	-	-	2.86	2.46
Br ⁻ (μg L ⁻¹)	46.77	-	-	49.10	-	-	16.49	46.88	-	27.48	-	-	-	-	44.04	23.83
I ⁻ (μg L ⁻¹)	ND	-	-	ND	-	-	ND	ND	-	ND	-	-	-	-	ND	ND
NH ₄ ⁺ (mg L ⁻¹)	-	-	-	-	-	-	<0.02	<0.02	<0.02	0.08	0.06	0.08	0.07	-	-	-
disinfectant	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂	Cl ₂
SW type	LR	LR	LR	LR	LR	LR	LR	LR	LR	LR	LR	GW	GW	GW	LR	LR

^a the number of the water treatment plant. ^b not detected. ^c not measured. ^d Lake and Reservoir. ^e Groundwater. ^f source water

TOC, Br⁻, I⁻, and NH₄⁺ were all detected in source water of the drinking water treatments.

Table S4. Concentrations of selected DBPs and their abundant species in drinking water samples of China ($\mu\text{g L}^{-1}$).

parameter	minimun	median	75th percentile	maximum
THM4	0.79	10.53	23.86	107.03
I-THMs	ND	ND	0.50	5.58
HAAs	0.45	10.95	17.79	59.64
DCAA	ND	3.93	7.21	52.85
TCAA	ND	3.97	6.91	16.33
HANs	ND	1.11	4.44	39.20
DCAN	ND	0.63	1.69	6.66
HNM _s	ND	0.05	0.12	0.96
CNM	ND	0.05	0.12	0.96
TCNM	ND	ND	ND	0.28

Table S5. The CHO toxic data of THMs from pervious study.¹⁻³

Chemical	CHO genotoxic potency (M)	CHO cytotoxicity %C _{1/2} value (M)
TIM	NS	6.60×10^{-5}
DBIM	NS	1.90×10^{-3}
DCIM	NS	4.13×10^{-3}
BCIM	NS	2.40×10^{-3}
TCM	NS	9.63×10^{-3}
BDCM	NS	1.12×10^{-2}
DBCM	NS	5.7×10^{-3}
TBM	NS	3.96×10^{-3}

THM4: The unit of genotoxicity index value =NS

The unit of cytotoxicity index value = 1.3×10^2

I-THMs: The unit of genotoxicity index value = NS

The unit of cytotoxicity index value = 1.3×10^3

Table S6. The CHO toxic data of HAAs from previous study.^{1,4}

Chemical	CHO genotoxic potency (M)	CHO cytotoxicity %C _{1/2} value (M)
BAA	1.7×10^{-5}	8.9×10^{-6}
DBAA	1.756×10^{-3}	5.0×10^{-4}
TBAA	2.456×10^{-3}	1.0×10^{-3}
CAA	4.1×10^{-4}	9.4×10^{-4}
DCAA	NS	1.14×10^{-2}
TCAA	NS	1.75×10^{-2}

HAAs: The unit of genotoxicity index value = 4.7×10^2

The unit of cytotoxicity index value = 1.03×10^3

Table S7. The CHO toxic data of HANs from previous study.⁵

Chemical	CHO genotoxic potency (M)	CHO cytotoxicity % C _{1/2} value (M)
IAN	3.71×10^{-5}	3.30×10^{-6}
BAN	3.85×10^{-5}	3.21×10^{-6}
DBAN	4.71×10^{-5}	2.85×10^{-6}
BCAN	3.24×10^{-4}	8.46×10^{-6}
CAN	6.01×10^{-4}	6.83×10^{-5}
DCAN	2.75×10^{-4}	5.73×10^{-5}
TCAN	1.01×10^{-3}	1.60×10^{-4}

HANs: The unit of genotoxicity index value = 3.6×10^3

The unit of cytotoxicity index value = 1.2×10^5

Table S8. The CHO toxic data of HNMs from previous study.⁶

Chemical	CHO genotoxic potency (M)	CHO cytotoxicity %C ½ value (M)
TBNM	6.99×10^{-5}	8.57×10^{-6}
CNM	2.15×10^{-3}	5.29×10^{-4}
TCNM	9.34×10^{-5}	5.36×10^{-4}
BCNM	1.65×10^{-4}	4.05×10^{-5}

HANs: The unit of genotoxicity index value = 1.0×10^4

The unit of cytotoxicity index value = 3.5×10^3

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