

Supplementary Information

Analysis of 13 haloacetamide DBPs in drinking water using a highly sensitive LC-MS/MS method

Table S1 Characteristics of the HAcAms Analyzed in this Study

No	HAcAms	Abbreviation	CAS ^a NO	Chemical Formula	MW ^b	Source and Purity
1	2-Chloroacetamide	CACAm	79-07-2	C ₂ H ₄ ClNO	93.51	Sigma-Aldrich,98%
2	2-Bromoacetamide	BACAm	683-57-8	C ₂ H ₄ BrNO	137.96	Sigma-Aldrich,98%
3	Iodoacetamide	IACAm	144-48-9	C ₂ H ₄ INO	184.96	Sigma-Aldrich,99%
4	2,2-Dichloroacetamide	DCACAm	683-72-7	C ₂ H ₃ Cl ₂ NO	127.96	J&K,98%
5	Trichloroacetamide	TCACAm	594-65-0	C ₂ H ₂ Cl ₃ NO	162.4	Sigma-Aldrich,99%
6	Diiodoacetamide	DIACAm	5875-23-0	C ₂ H ₃ I ₂ NO	310.85	CanSyn Chem Corp.,> 99%
7	Tribromoacetamide	TBACAm	594-47-8	C ₂ H ₂ Br ₃ NO	295.75	CanSyn Chem Corp.,> 99%
8	Bromiodoacetamide	BIIACAm	62872-36-0	C ₂ H ₃ BrINO	263.856	CanSyn Chem Corp.,> 85%
9	Dibromochloroacetamide	DBCACAm	855878-13-6	C ₂ H ₂ Br ₂ ClNO	251.305	CanSyn Chem Corp.,> 99%
10	Chloriodoacetamide	CIACAm	62872-35-9	C ₂ H ₃ ClINO	219.405	CanSyn Chem Corp.,> 99%
11	Bromodichloroacetamide	BDCACAm	98137-00-9	C ₂ H ₂ BrCl ₂ NO	206.85	CanSyn Chem Corp.,> 99%
12	Dibromoacetamide	DBACAm	598-70-9	C ₂ H ₃ Br ₂ NO	216.86	CanSyn Chem Corp.,> 99%
13	Bromochloroacetamide	BCACAm	62872-34-8	C ₂ H ₃ BrClNO	172.41	CanSyn Chem Corp.,> 99%

^a CAS = chemical abstracts service; ^b MW = molecular weight;

Table S2 Detailed information of 15 WTPs considered in this study

WTPs	District	Water source	Advanced treatment (ozone-BAC process)	Disinfectant
WTP1	Wuxi	Yangtze River	Yes	chlorine
WTP2	Wuxi	Taihu Lake	Yes	chlorine
WTP3	Wuxi	Taihu Lake	Yes	chlorine
WTP4	Wuxi	Taihu Lake	Yes	chlorine
WTP5	Jiangyin	Yangtze River	No	chlorine
WTP6	Jiangyin	Yangtze River	No	chlorine
WTP7	Jiangyin	Yangtze River	No	chlorine
WTP8	Yixing	Hengshan Reservoir	No	chlorine
WTP9	Yixing	Dahanjie Reservoir	No	chlorine
WTP10	Yixing	Longzhu Reservoir	No	chlorine
WTP11	Yixing	Hengshan Reservoir	Yes	chlorine
WTP12	Yixing	Youche Reservoir	No	chlorine
WTP13	Kunshan	Kuilei Lake	No	Chloramine
WTP14	Kunshan	Kuilei Lake	No	Chloramine
WTP15	Kunshan	Kuilei Lake	No	Chloramine

Table S3 Precision and accuracy of this method

Analyte	LOD ($\mu\text{g L}^{-1}$)	LOQ ($\mu\text{g L}^{-1}$)	Target concentration ($\mu\text{g L}^{-1}$)	Intra-day ($n = 6$)			Inter-day ($n = 3$)		
				Obtained concentration ($\mu\text{g L}^{-1}$)	Accuracy (%)	Precision (%)	Obtained concentration ($\mu\text{g L}^{-1}$)	Accuracy (%)	Precision (%)
CAcAm	0.010	0.030	0.500	0.491±0.010	98.2	2.6	0.484±0.020	96.8	4.1
			1.000	0.995±0.013	99.5	1.6	0.973±0.015	97.3	3.2
			10.0	8.940±0.10	89.4	1.4	9.02±0.12	90.2	2.8
BAcAm	0.010	0.030	0.500	0.445±0.008	89.0	2.7	0.442±0.016	88.4	3.5
			1.000	0.941±0.014	94.1	1.7	0.918±0.015	91.8	2.6
			10.0	9.130±0.09	91.3	1.1	9.05±0.11	90.5	2.0
IAcAm	0.002	0.006	0.500	0.515±0.012	103	2.4	0.505±0.020	101	3.8
			1.000	1.120±0.015	112	1.7	1.09±0.018	109	2.5
			10.0	9.180±0.09	91.8	1.2	8.98±0.10	89.8	2.2
DCAcAm	0.020	0.060	0.500	0.590±0.013	118	2.8	0.56±0.024	112	4.9
			1.000	1.060±0.018	106	2.1	1.010±0.023	101	3.5
			10.0	8.460±0.08	84.6	1.5	8.53±0.14	85.3	2.7
CBAcAm	0.010	0.030	0.500	0.486±0.010	97.2	2.8	0.478±0.014	95.6	3.3
			1.000	0.968±0.008	96.8	1.6	0.957±0.012	95.7	2.4
			10.0	8.720±0.10	87.2	1.2	8.61±0.12	86.1	2.1
DBAcAm	0.020	0.060	0.500	0.475±0.009	95.0	2.9	0.471±0.012	94.2	3.4
			1.000	1.070±0.015	107	2.5	1.04±0.018	104	2.8
			10.0	9.470±0.09	94.7	1.5	9.33±0.11	93.3	2.2
CIAcAm	0.002	0.006	0.500	0.423±0.010	84.6	2.4	0.414±0.020	82.8	3.9
			1.000	1.080±0.016	108	2.0	1.05±0.018	105	2.8
			10.0	8.980±0.11	89.8	1.1	9.04±0.15	90.4	2.5

			0.500	0.515±0.011	103	2.1	0.505±0.018	101	3.6
BIAcAm	0.003	0.009	1.000	1.080±0.013	108	1.9	1.05±0.018	105	2.9
			10.0	10.680±0.08	107	1.7	10.19±0.09	102	2.2
			0.500	0.475±0.013	95.0	2.6	0.484±0.015	96.8	3.2
DIAcAm	0.001	0.003	1.000	1.170±0.012	117	2.3	1.13±0.015	113	2.9
			10.0	9.90±0.08	99.0	1.9	9.75±0.09	97.5	2.4
			0.500	0.435±0.011	87.0	3.6	0.431±0.019	86.2	5.0
TCAcAm	0.001	0.003	1.000	0.905±0.015	90.5	1.8	0.906±0.016	90.6	2.3
			10.0	9.960±0.09	99.6	1.3	9.511±0.09	95.1	2.0
			0.500	0.487±0.010	97.4	2.9	0.479±0.019	95.8	4.3
BDCAcAm	0.002	0.006	1.000	0.902±0.009	90.2	1.8	0.884±0.015	88.4	3.5
			10.0	8.920±0.10	89.2	1.3	8.65±0.11	86.5	2.3
			0.500	0.535±0.011	107	2.6	0.52±0.020	104	3.7
DBCcAm	0.003	0.009	1.000	0.866±0.012	86.6	1.6	0.854±0.017	85.4	3.1
			10.0	8.520±0.08	85.2	1.2	8.402±0.12	84	2.6
			0.500	0.540±0.013	108	3.2	0.525±0.025	105	5.7
TBAcAm	0.100	0.300	1.000	1.110±0.020	111	2.6	1.07±0.020	107	3.4
			10.0	9.020±0.08	90.2	1.1	8.68±0.10	86.8	3

Table S4 MRM parameters of 13 HAcAms

HAcAm	Precursor Ions (m/z)	Daughter Ions (m/z)	DP (V)	CE (V)	CXP (V)
CAcAm	94	58.1	80	18	8
	94	77	80	20	8
BAcAm	138	59.1	60	26	7
	140	59	60	24	7
CBAcAm	171.9	92.9	60	23	10
	174	93	50	24	10
IAcAm	186	59.1	45	21	9
	186	43	45	51	9
DBAcAm	218	137	95	24	10
	218	107.9	95	33	10
CIAcAm	220	93	40	19	15
BIAcAm	263.9	137	65	27	23
	265.9	139	65	27	23
TBAcAm	295.8	216.9	30	28	8
	297.8	217	30	27	8
DIAcAm	311.9	184.9	45	24	10
	311.9	167.9	45	43	10
DCAcAm	128	64.1	60	24	10
	128	92	60	17	10
TCAcAm	159.9	116.9	-35	-13	-15
BDCAcAm	205.8	162.8	-30	-12	-16
	205.8	42	-30	-14	-16
DBCacAm	249.8	206.8	-20	-12	-12
	249.8	78.9	-20	-28	-12

Table S5 Comparison of HAcAms in drinking water disinfected by different disinfection agents ($\mu\text{g L}^{-1}$)

HAcAms	Mean \pm SD		P^a	Medium(P25,P75)		P^c
	Chlorination n	Chloramination ion		Chlorination	Chloramination	
CAcAm	0.0434 \pm 0.0 030	0.2918 \pm 0.06 91	7.15 $\times 10^{-10}$	0.041(0.027,0.0 57)	0.179(0.099,0. 562)	5.91 $\times 10^{-6}$
BacAm	0.0182 \pm 0.0 017	0.0568 \pm 0.00 44	1.42 $\times 10^{-11}$	0.016(0.013,0.0 24)	0.058(0.050,0. 068)	3.28 $\times 10^{-5}$
CBAcAm	0.2987 \pm 0.0 451	0.7367 \pm 0.11 29	1.13 $\times 10^{-4}$	0.156(0.084,0.0 398)	0.916(0.378,1. 030)	0.0027
IAcAm	0.0158 \pm 0.0 072	0.1209 \pm 0.01 99	4.30 $\times 10^{-6}$	0.004(0.002,0.0 14)	0.090(0.068,0. 178)	0.0003
DBAcAm	0.0973 \pm 0.0 177	0.3540 \pm 0.05 73	4.71 $\times 10^{-7}$	0.051(0.003,0.1 41)	0.420(0.190,0. 523)	0.0002
CIAcAm	0.0191 \pm 0.0 056	0.0475 \pm 0.01 02	0.0116	0.011(0.002,0.0 18)	0.049(0.018,0. 065)	0.0059
BIAcAm	0.0037 \pm 0.0 027	0.0060 \pm 0.00 50	0.68	0.002(0,0.009)	0.006(0.001,0. 011)	0.5637
TBAcAm	0.1086 \pm 0.0 135	0.0933 \pm 0.01 31	0.6016	0.091(0.057,0.1 44)	0.082(0.069,0. 108)	0.9502
DIAcAm	0.0136 \pm 0.0 052	0.0073 \pm 0.00 46	0.3979	0.009(0.001,0.0 29)	0.002(0.002,0. 006)	0.8973
DCAcAm	0.6333 \pm 0.0 756	1.892 \pm 0.329 5	4.35 $\times 10^{-7}$	0.480(0.203,0.9 75)	1.872(0.714,2. 911)	0.0006
TCAcAm	ND ^b	ND ^b	ND ^b	ND ^b	ND ^b	ND ^b
DCBAcAm	0.0808 \pm 0.0 040	0.0973 \pm 0.00 99	0.072	0.073(0.065,0.0 92)	0.077(0.072,0. 115)	0.0709
CDBAcAm	0.0198 \pm 0.0 098	0.0393 \pm 0.00 97	0.2071	0.013(0.008,0.0 20)	0.043(0.025,0. 054)	0.1416
Total	1.239 \pm 0.12 79	3.6033 \pm 0.56 82	5.10 $\times 10^{-8}$	0.894(0.546,1.8 70)	4.069(1.711,5. 252)	0.0003

^a Student t-test.

^b no value

^c Kruskal-Wallis test