Supporting Information

Simultaneous prediction of trihalomethanes, haloacetic acids, haloacetonitriles and haloacetamides using simulated distribution system tests

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Table S1: Extraction and gas chromatography specifications and operational conditions in modified EPA Method 551.1, for THMs, HANs and HAcAms.

Extraction:	Liquid-liquid extraction (LLE) with MTBE Internal standard: bromofluorobenzene [1 µg/ml]
Primary Column:	RXi 5Sil MS, 30m · 0.25mm ID, 0.25 µm film thickness
Injector:	Injector temperature –170 °C; 2 mm straight quartz liner; injection volume 1 µL; splitless injection hold for 45 seconds then purge at 30 mL/min.
Carrier Gas:	Helium (*set at constant pressure*), velocity 33 cm/sec.
GC program:	▪ HOLD at 35°C for 22 minutes. ▪ INCREASE to 145°C at 10°C/min and hold at 145°C for 2 minutes. ▪ INCREASE to 225°C at 20°C/min and hold at 225°C for 15 minutes. ▪ INCREASE to 260°C at 10°C/min and hold at 260°C for 30 minutes.
Total time: 90 min/ sample	
Detector:	Agilent Micro ECD (150 µL); Detector temperature: 290 °C; Make up gas: 99.9% nitrogen at 30 mL/min.

Table S2: Extraction and gas chromatography specifications, and operational conditions in EPA Method 552.3 for HAAs.

Extraction:	Liquid-liquid extraction (LLE) with MTBE, and derivatization via methylation Internal standard: 1,2,3-trichloropropane [1 µg/ml]
Primary column:	DB-1701, 30m · 0.25mm ID, 0.25 µm firm thickness.
Injector:	Injector temperature – 210°C; 2 mm straight quartz liner; injection volume 1 µL; splitless injection hold for 45 seconds then purge at 30 mL/min.
Carrier Gas:	Helium (set at constant pressure), velocity 33 cm/sec.
GC program:	▪ HOLD at 40°C for 10 minutes. ▪ INCREASE to 65°C at 2.5°C/min. ▪ INCREASE to 85°C at 10°C/min. ▪ INCREASE to 205°C at 20°C/min, and hold at 205°C for 7 minutes.
Total time: 35 min/ sample	
Detector:	Agilent Micro ECD (150 µL); detector temperature: 290 °C; Make up gas: 99.9% nitrogen at 20 mL/min.

Table S3: DBP monitoring in numbers (MDL, recovery rate, n° of samples, median concentrations).

Target Analyte		**MDL** [µg/L]	**Recovery rate** [%]	**Total samples** [n°]	**Samples >MDL** [n°]	**Median concentration** [µg/L]
THMs	Chloroform	0.4	108	384	384	4.8
	Bromodichloromethane	0.3	110	384	384	6.8
	Dibromochloromethane	0.2	110	384	384	10.8
	Bromoform	0.4	98	384	376	7.7
HAAs	Monochloroacetic acid	0.2	95.8	374	320	3.3
	Monobromoacetic acid	0.5	92.2	374	358	1.4
	Dichloroacetic acid	0.2	93.8	374	324	4.4
	Trichloroacetic acid	0.2	105	374	364	0.9
	Bromochloroacetic acid	0.1	98	374	96	2.6
	Bromodichloroacetic acid	0.1	101	374	340	1.7
	Dibromoacetic acid	0.7	110	374	338	2.5
	Dibromochloroacetic acid	1	108	374	338	3.2
	Tribromoacetic acid	1	90.6	374	320	2.9
HANs	Dichloroacetonitrile	0.1	90	380	308	0.6
	Trichloroacetonitrile	0.1	95	380	302	0.7
	Dibromoacetonitrile	0.2	95	380	266	0.8
	Bromochloroacetonitrile	0.2	110	380	312	0.6
	Monochloroacetonitrile	-	n/a	380	n/a	n/a
	Monobromoacetonitrile	0.1	90	380	82	0.1
	Dibromochlroacetonitrile	0.5	95	380	0	n/a
HAcAms	Monochloroacetamide	-	n/a	372	n/a	n/a
	Monobromoacetamide	0.1	70	372	244	0.6
	Dichloroacetamide	0.1	85	372	368	0.8
	Trichloroacetamide	0.1	80	372	260	0.3
	Dibromoacetamide	0.1	88	372	350	0.6
	Bromochloroacetamide	0.1	73	372	326	0.8
	Bromodichloroacetamide	0.1	70	372	306	0.3
	Dibromochlroacetamide	0.1	71	372	190	0.3
	Tribromoacetamide	0.1	70	372	280	0.3

Table S4: Summary of water quality characteristics range of the chlorinated and chloraminated SDS tests (between 6-106 hours) during the seasonal samplings.

WTW	**Units**	**A**				**B**				**C**				**D**			
Sampling rounds		Autumn	Winter	Spring	Summer	Autumn	Winter	Spring	Summer	Autumn	Winter	Spring	Summer	Autumn	Winter	Spring	Summer
Disinfectant type	-	Chlorination				Chlorination				Chloramination				Chloramination			
Disinf. residual	mg/L Cl_2	0.9-0.2	0.7-0.2	1.0-0.2	1.1-0.3	0.6-0.2	0.6-0.3	0.6-0.4	1.1-0.4	1.2-0.9	1.0-0.3	0.9-0.5	1.0-0.5	0.6-0.2	0.8-0.6	1.0-0.2	1.0-0.2
Water temperature	°C	17.0	8.0	14.0	20.0	17.0	8.0	14.0	20.0	14.0	8.0	17.0	20.0	14.0	8.0	17.0	20.0
TOC	mg/L C	3.1-3.7	3.1-3.6	3.3-3.5	2.9-3.9	3.8	3.2-3.6	3.5-4.1	3.7-3.5	3.1-4.0	3.3-3.4	3.2-3.4	2.1-3.0	2.8-3.3	2.5-2.8	1.8-1.9	2.7-3.0
pH	-	7.2	7.5-7.9	7.0-7.5	7.0-7.1	n/a	7.2-7.7	7.0-7.7	7.2	6.9-7.3	7.6-7.7	7.4-7.6	7.4-7.5	6.5-7.3	7.3-7.5	7.3-7.5	7.5
Bromide	µg/L	<12.0	<12.0	<12.0	<12.0	<12.0	18.3	<12.0	12.0	82	85.1	76	80.0	13.2	19.9	26.4	<12.0
UV_{abs}	1/M·cm	n/a	0.04-0.06	0.06	n/a	n/a	0.04-0.06	0.04-0.07	n/a	n/a	0.06	0.04	0.05-0.06	0.03-0.05	0.06	0.04	0.05
SUVA	-	n/a	1.2-1.6	1.8	n/a	n/a	1.2-1.9	1.1-1.6	n/a	n/a	1.7	1.4	2.3-2.6	1.0-1.7	2.1-2.3	2.2-2.3	1.9

Table S5: Key concept and equation of the weight ratios [%].

The weight ratios [%], also referred as mass percent composition, can be abbreviated as w/w %. This is a type of generic calculation that enables us to assess the ratio of specific species/sub-species against the sum of a category. In DBP analysis, the weight ratio term is usually calculated to assess the contribution of brominated species of a specific class to the sum of species (total). Also, this calculation was used to calculate the contribution of HAA5 against HAA9. In this study the following equation was used to calculate the weight ratios:

Weight-Ratio [%] = Concentration of sub-category [mg/L] / Concentration of category (*total*) [mg/L] × 100

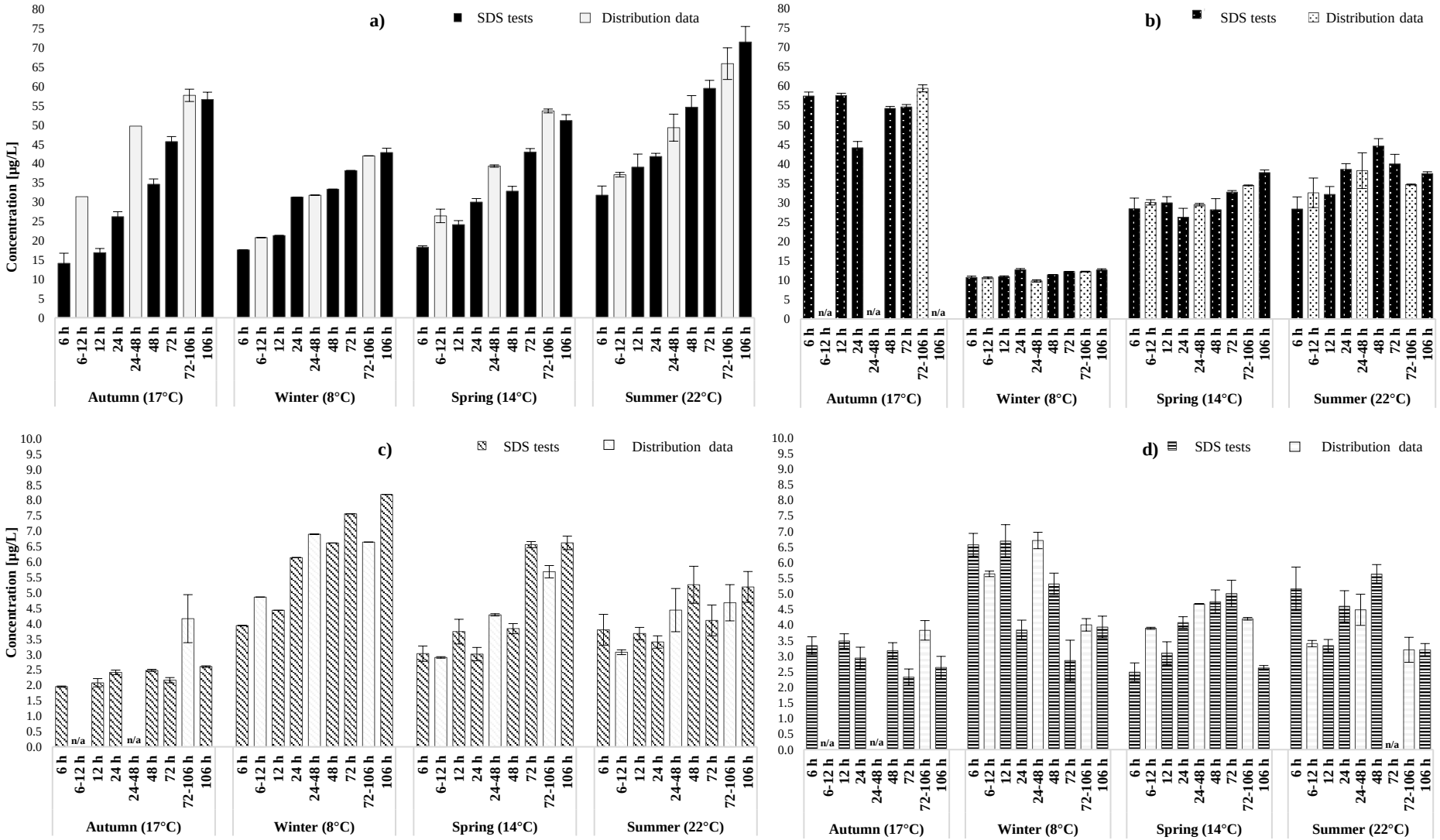

Figure S1: DBP occurrence of **a)** THMs, **b)** HAAs, **c)** HANs and **d)** HAcAms from SDS tests (*6, 12, 24, 48, 72, 106 hours*) and actual distribution samples (*6-12, 24-48, 72-106 hours*) in **chlorinated** water treatment works **B** (*4 seasonal rounds*).

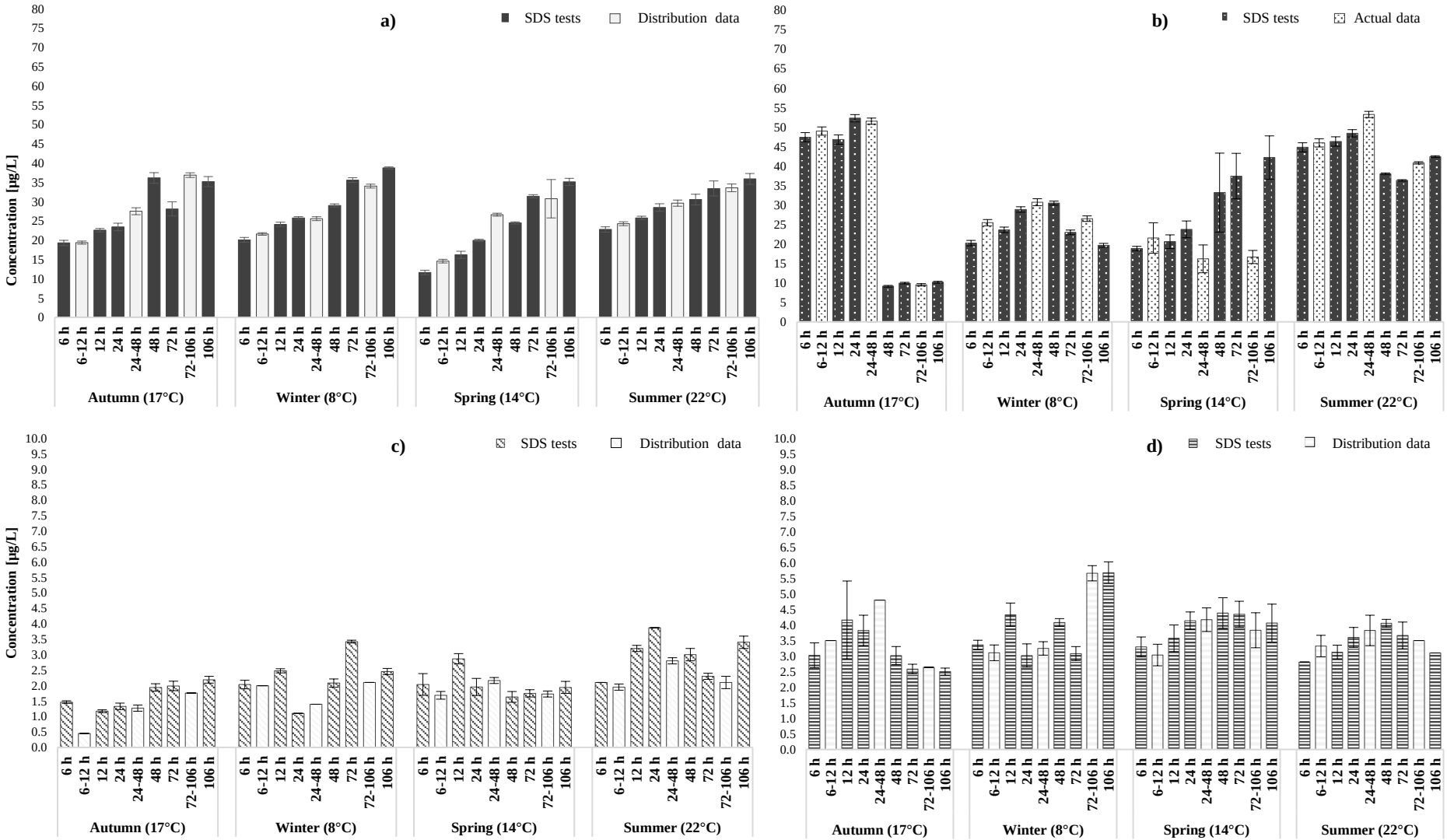

Figure S2: DBP occurrence of **a)** THMs, **b)** HAAs, **c)** HANs and **d)** HAcAms from SDS tests (*6, 12, 24, 48, 72, 106 hours*) and actual distribution samples (*6-12, 24-48, 72-106 hours*) in **chloraminated** water treatment works **D** (*4 seasonal rounds*).