

## Electronic Supplementary Information

# Molecular changes among non-volatile disinfection by-products between drinking water treatment and consumer taps

Anna Andersson<sup>a\*</sup>, Michael Gonsior<sup>b</sup>, Mourad Harir<sup>c,d</sup>, Norbert Hertkorn<sup>c</sup>, Philippe Schmitt-Kopplin<sup>c,d</sup>, Leanne Powers<sup>b</sup>, Henrik Kylin<sup>a,e</sup>, Daniel Hellström<sup>f</sup>, Kerstin Nilsson<sup>g</sup>, Ämma Pettersson<sup>h</sup>, Helena Stavklint<sup>i</sup> and David Bastviken<sup>a</sup>

<sup>a</sup> Department of Thematic Studies – Environmental Change, Linköping University, SE-581 83 Linköping, Sweden

<sup>b</sup> University of Maryland Center for Environmental Science, Chesapeake Biological Laboratory, Solomons, Maryland 20688, USA

<sup>c</sup> Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München, German Research Center for Health and Environment, Ingolstaedter Landstraße 1, 85764 Neuherberg, Germany

<sup>d</sup> Chair of Analytical Food Chemistry, Technische Universität München, 85354 Freising, Germany

<sup>e</sup> Research Unit: Environmental Sciences and Management, North-West University, Potchefstroom, South Africa

<sup>f</sup> Norrvatten, Kvalitet och Utveckling, SE-169 02 Solna, Sweden

<sup>g</sup> VA SYD, Rännemästaregatan 3, SE-212 23 Malmö, Sweden

<sup>h</sup> Nodra, Borgs vattenverk, SE-603 36 Norrköping, Sweden

<sup>i</sup> Tekniska verken i Linköping AB (publ), SE-581 15 Linköping, Sweden

\*Corresponding author: [anna.e.andersson@liu.se](mailto:anna.e.andersson@liu.se)

LIN      Mar ■      May ■      Aug ■      Nov ■      Jan ■

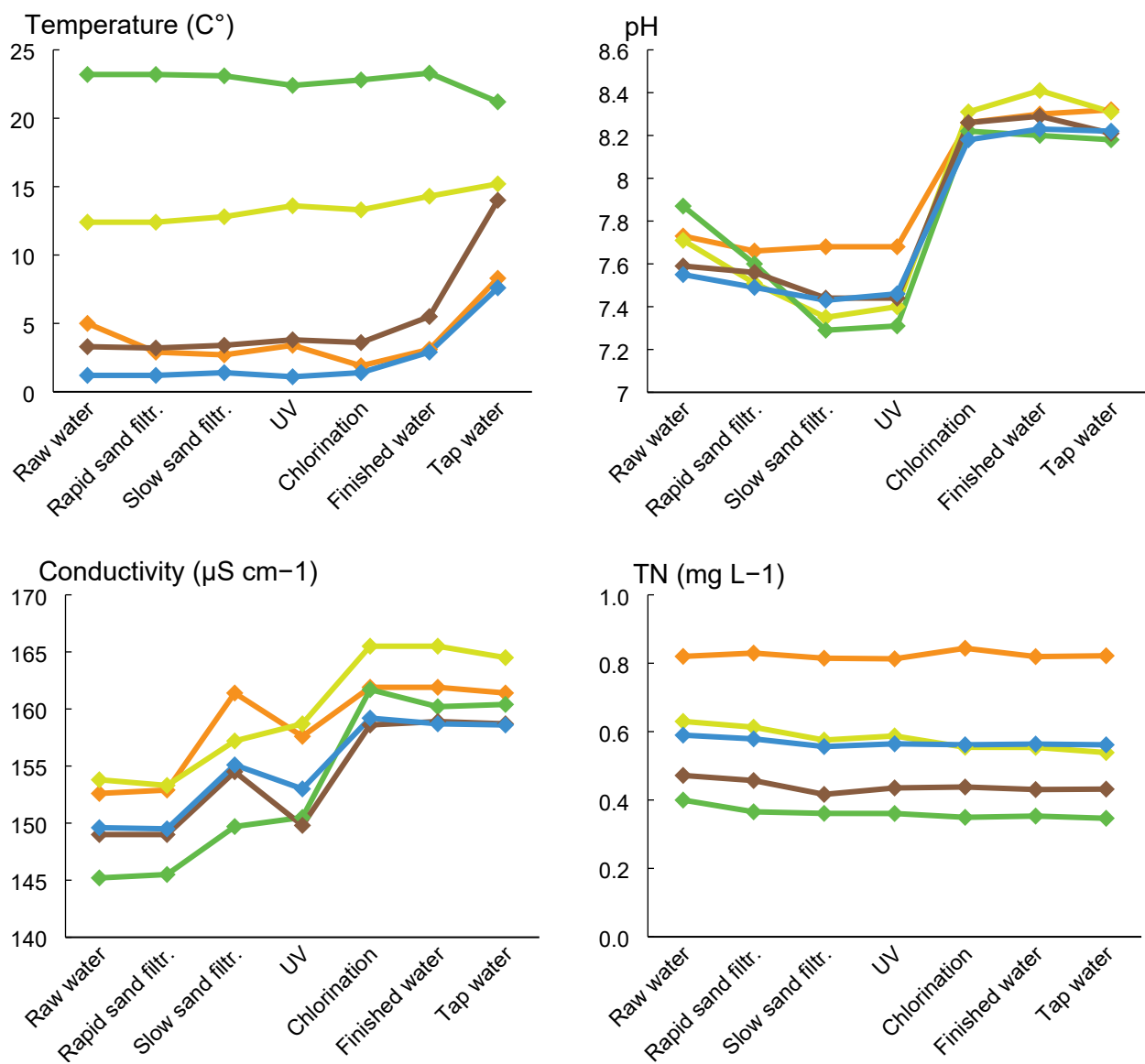
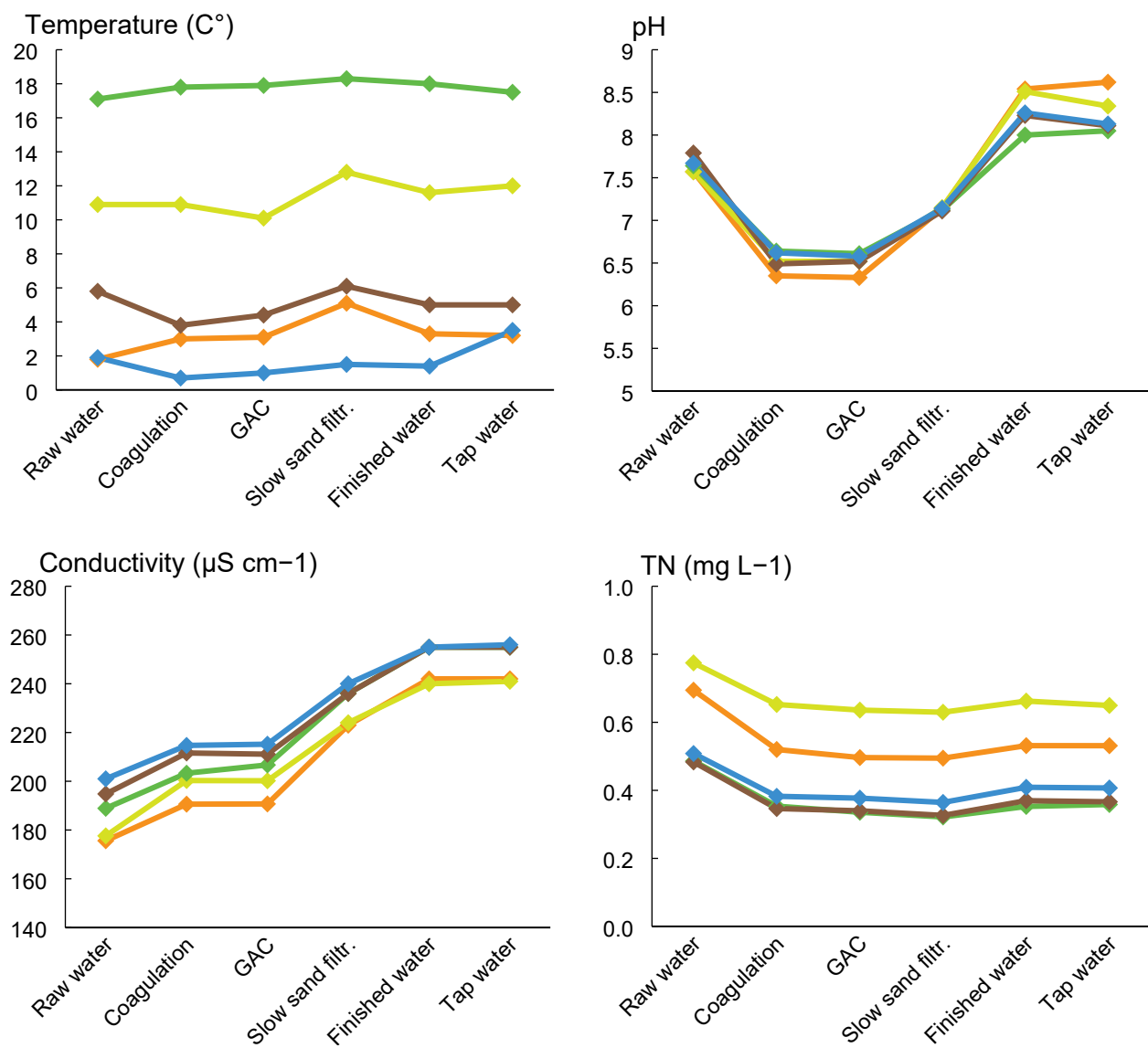


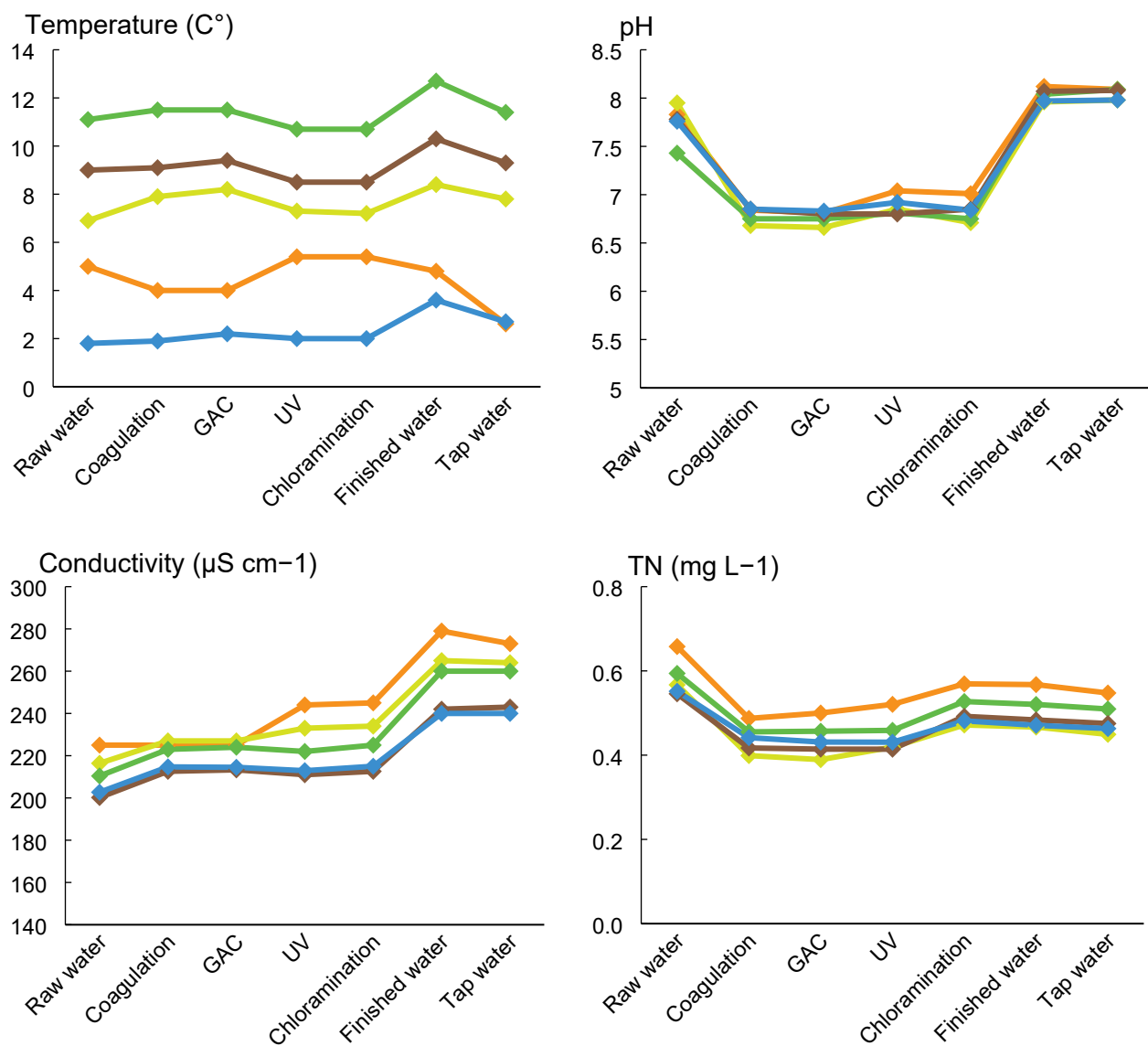
Figure S1. Changes in temperature, pH, conductivity, and total nitrogen (TN) upon treatment at LIN.

# NOR



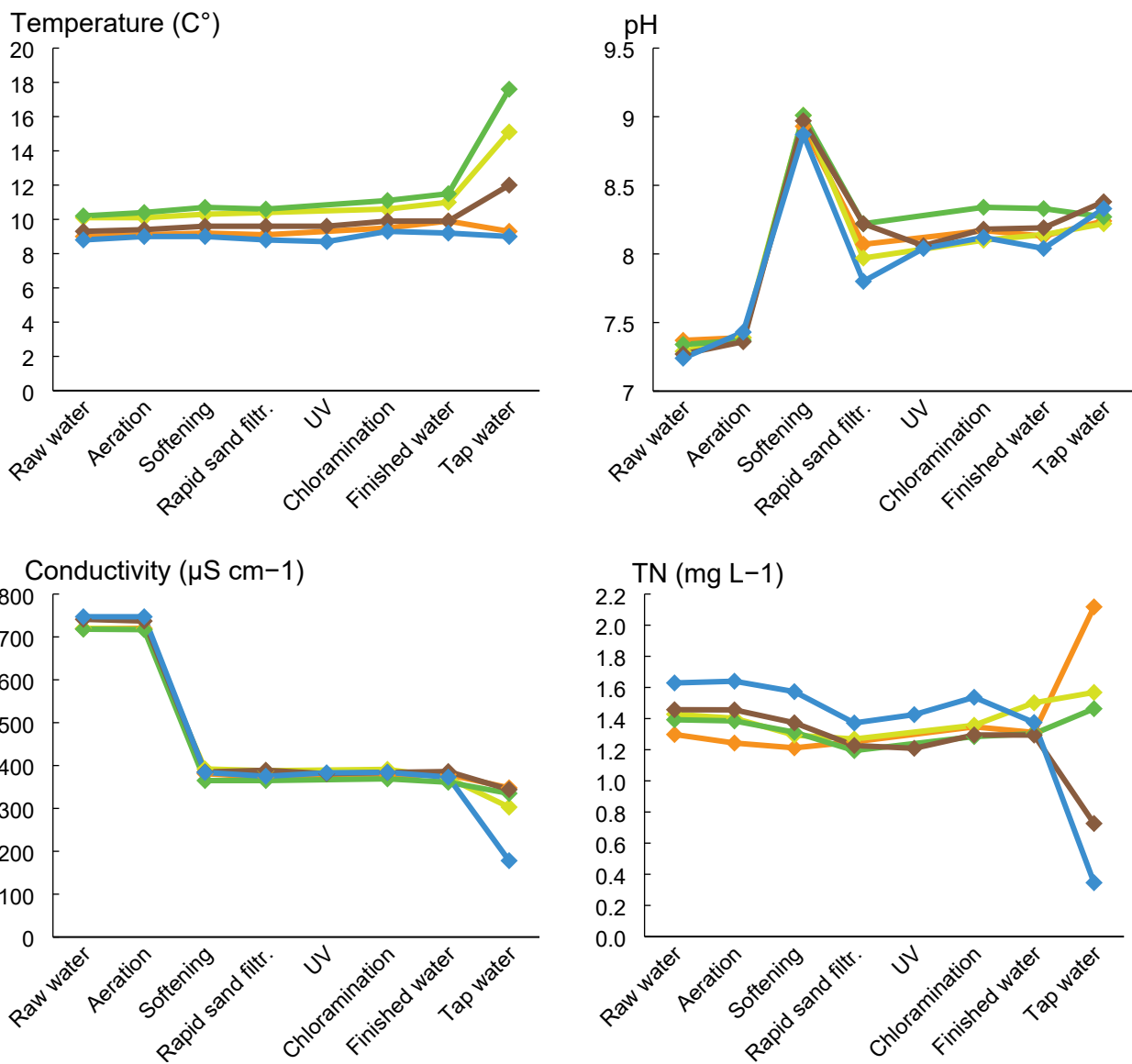
**Figure S2.** Changes in temperature, pH, conductivity, and total nitrogen (TN) upon treatment at NOR.

# STO



**Figure S3.** Changes in temperature, pH, conductivity, and total nitrogen (TN) upon treatment at STO.

# MAL



**Figure S4.** Changes in temperature, pH, conductivity, and total nitrogen (TN) upon treatment at MAL. UV was installed during the sample campaign, why data at this sampling point are available for two occasions only.

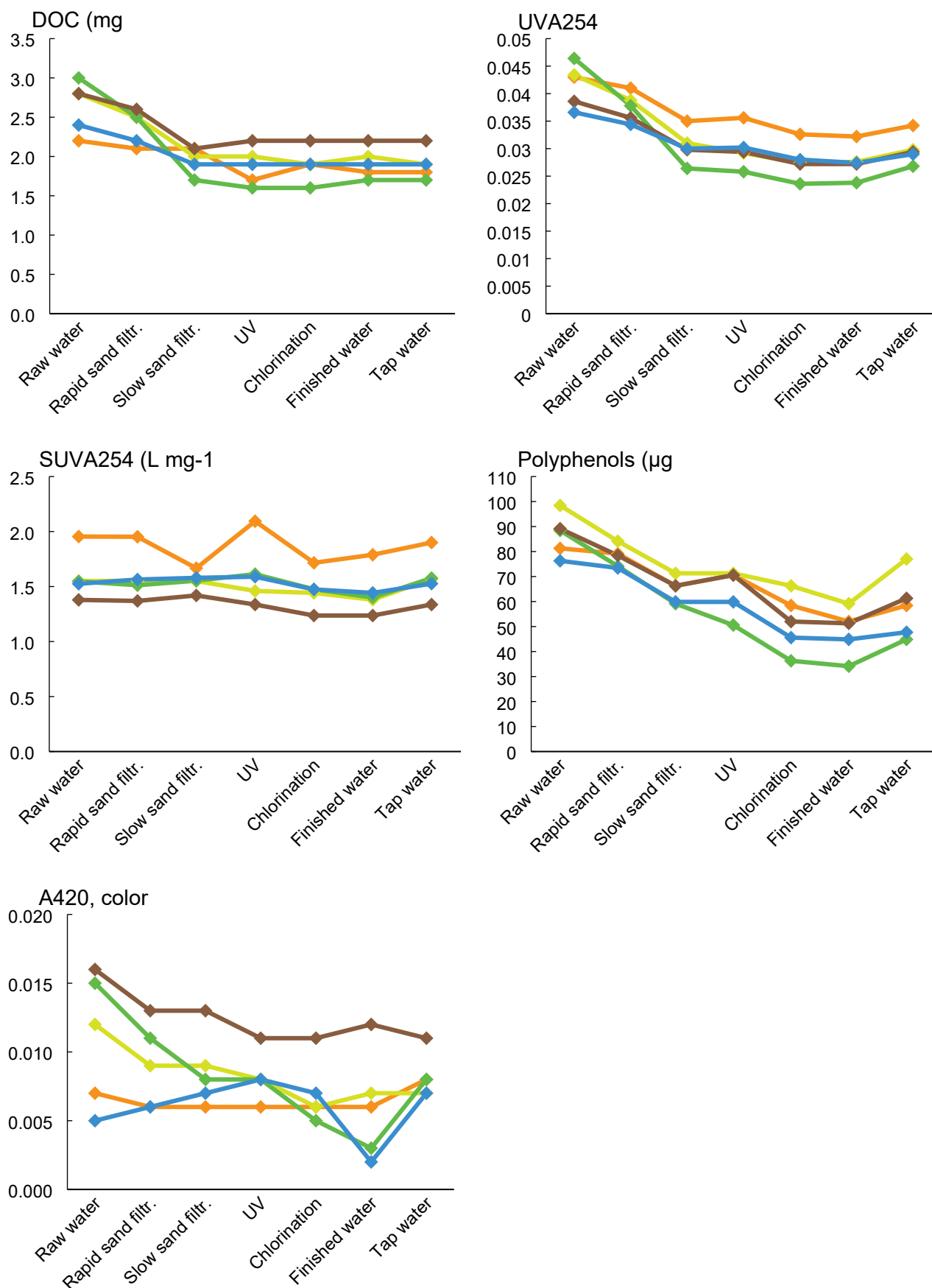
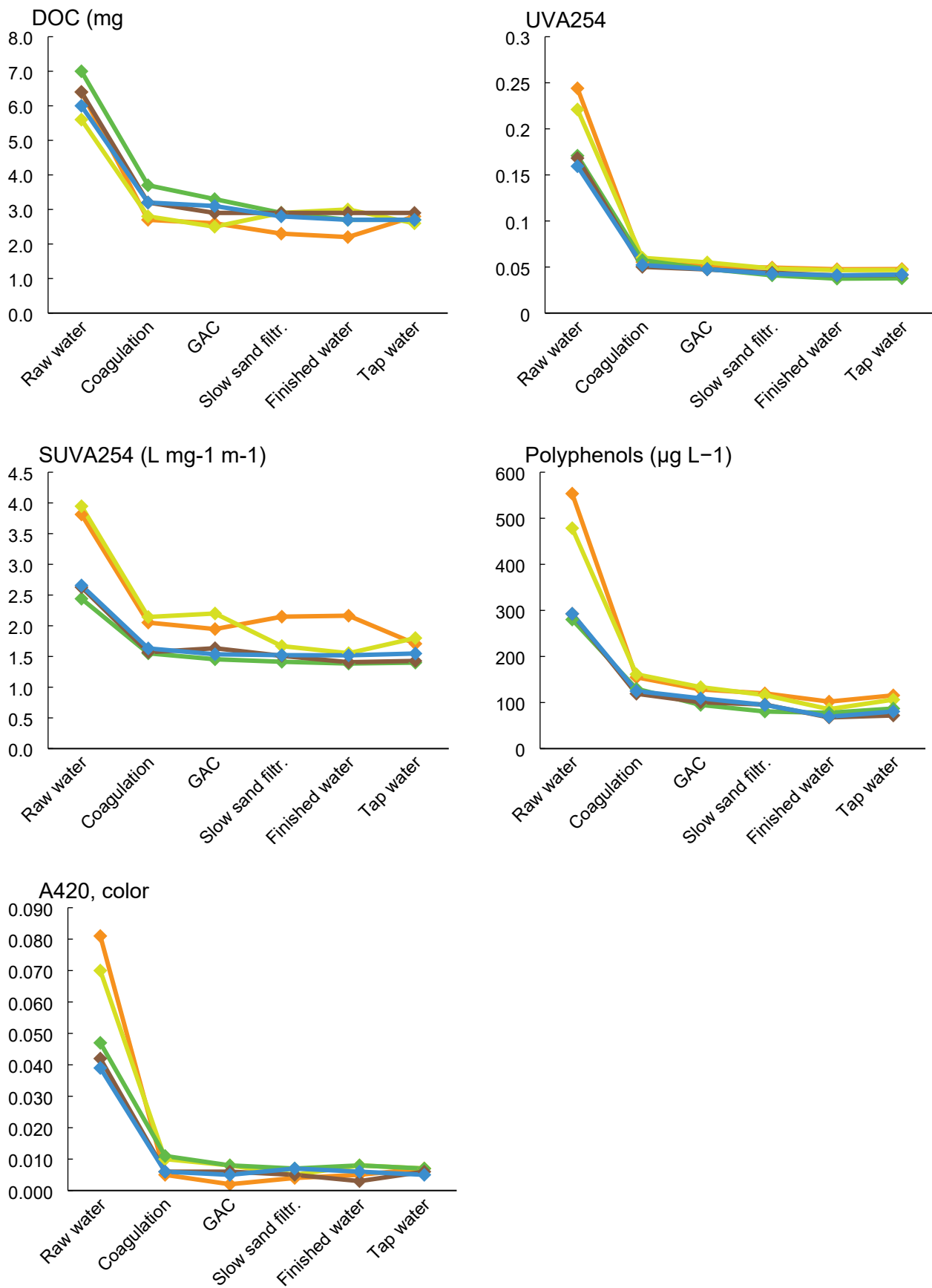


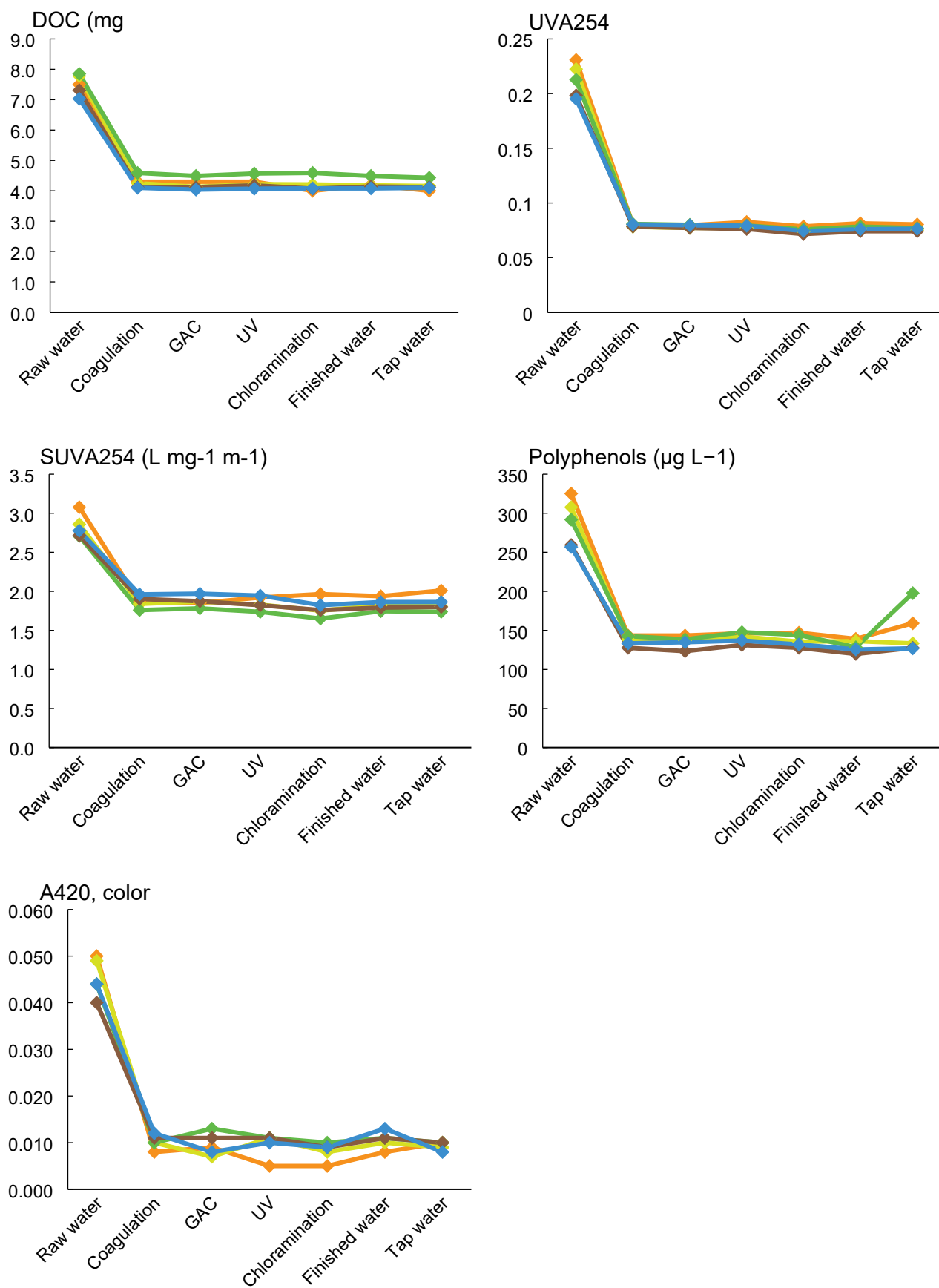
Figure S5. Changes in DOC, UVA<sub>254</sub>, SUVA<sub>254</sub>, polyphenols and A<sub>420</sub> upon treatment at LIN.

# NOR



**Figure S6.** Changes in DOC, UVA<sub>254</sub>, SUVA<sub>254</sub>, polyphenols and A<sub>420</sub> upon treatment at NOR.

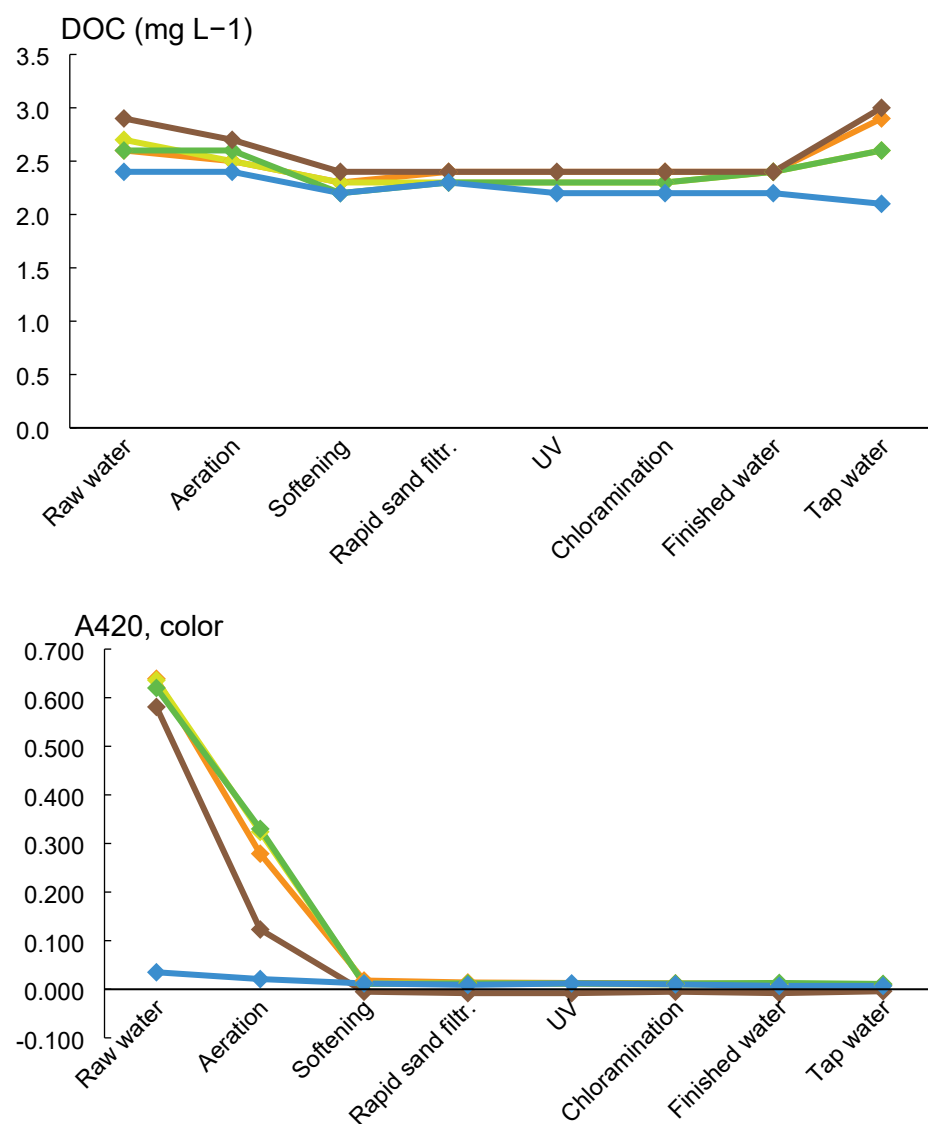
# STO



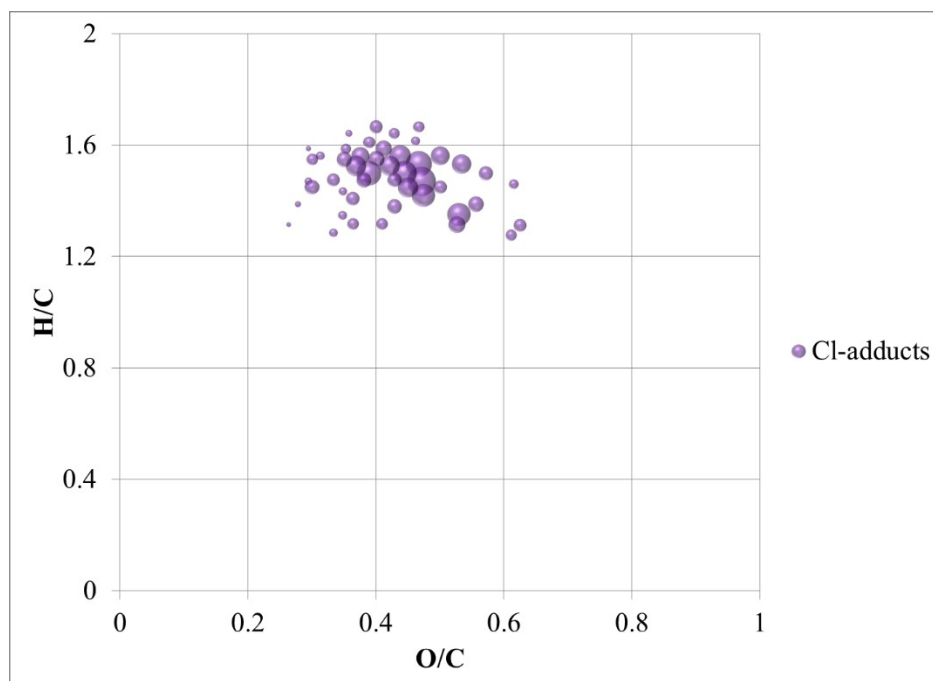
**Figure S7.** Changes in DOC, UVA<sub>254</sub>, SUVA<sub>254</sub>, polyphenols and A<sub>420</sub> upon treatment at STO.



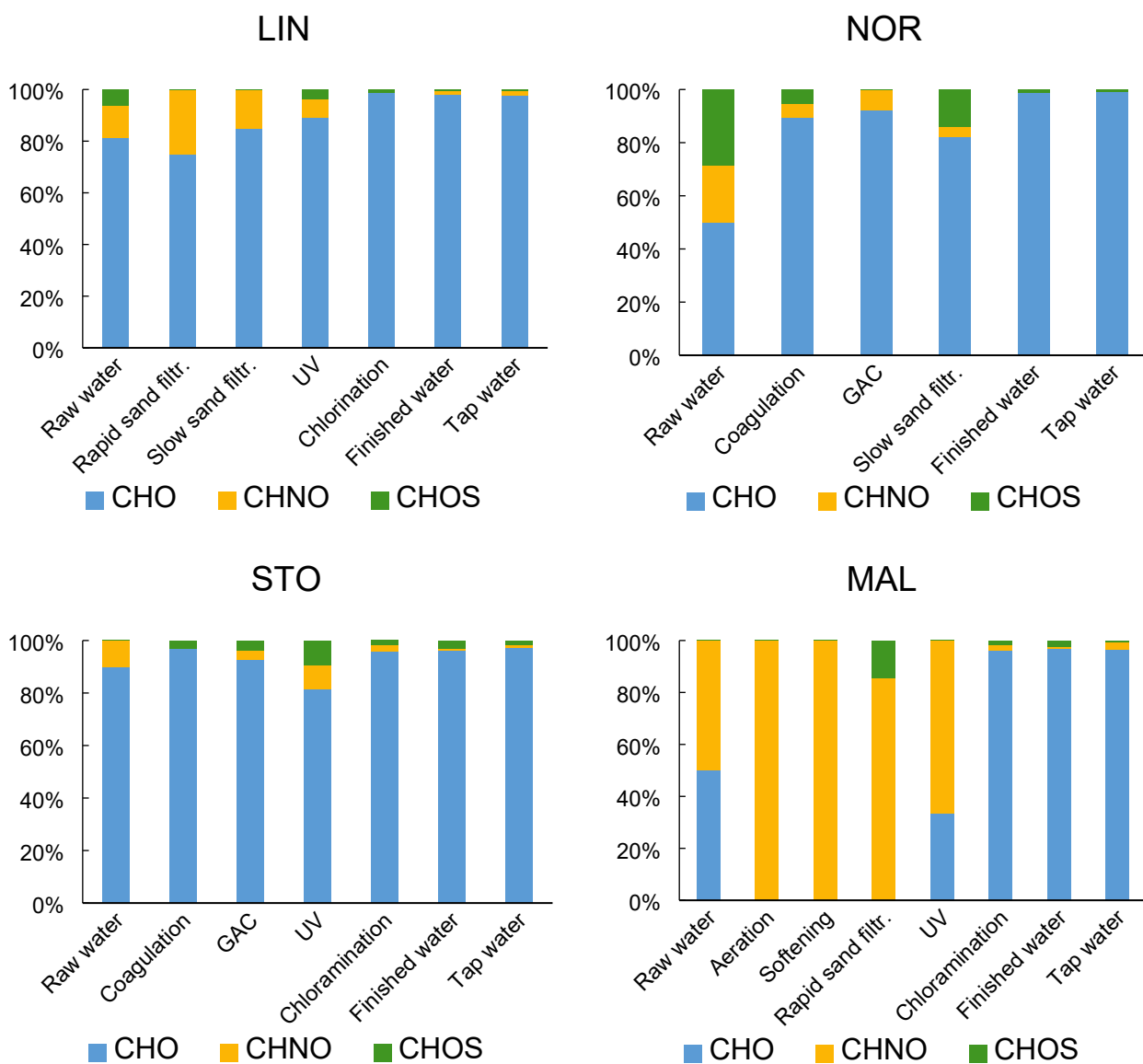
# MAL



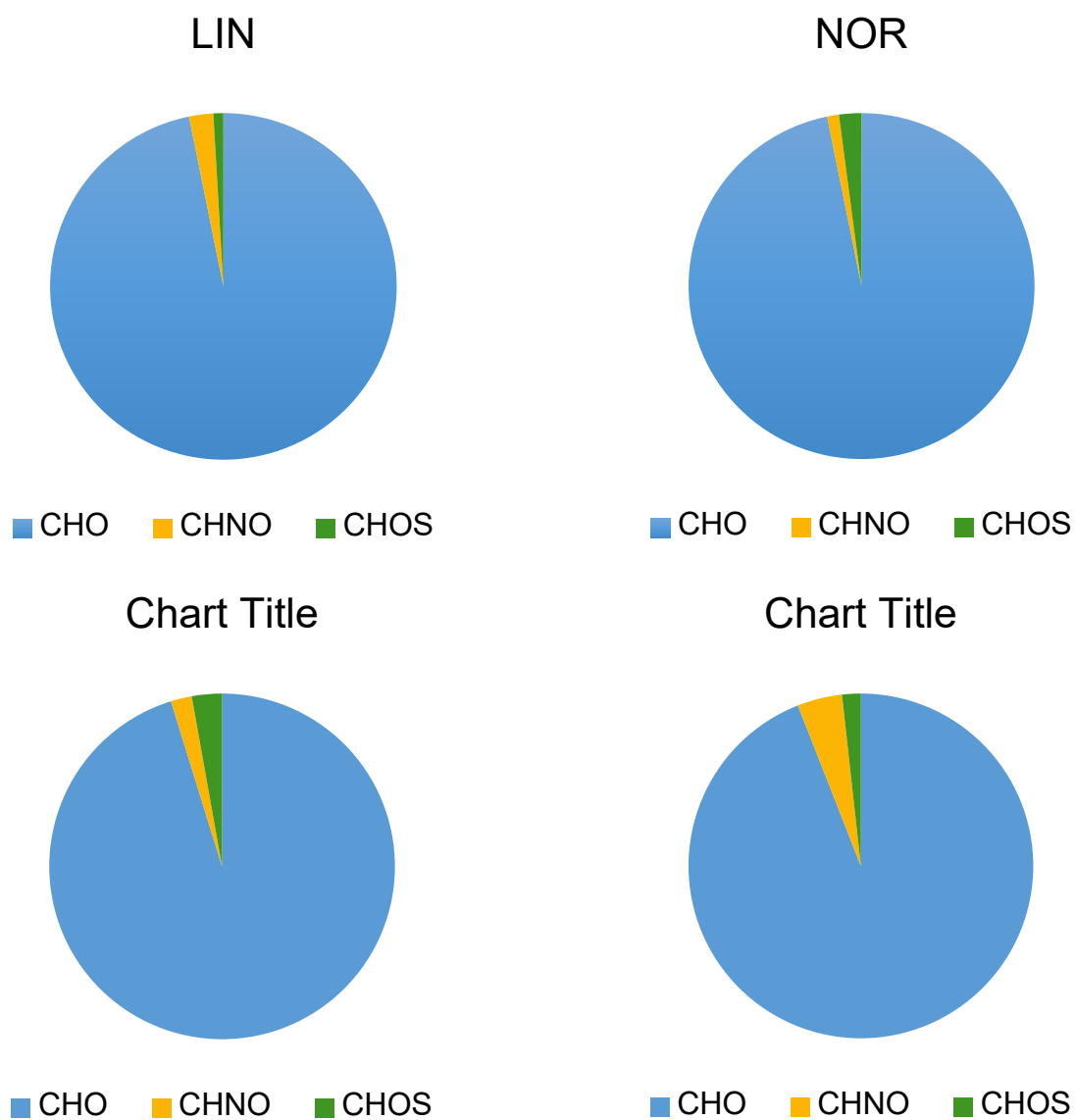
**Figure S8.** Changes in DOC and A<sub>420</sub> upon treatment at MAL. Data for UVA<sub>254</sub>, SUVA<sub>254</sub>, and polyphenols are not shown due to interferences of iron on absorbance measurements for DOM analysis at this water source. UV was installed during the sample campaign, why data at this sampling point only are available for two occasions.



**Figure S9.** Van Krevelen diagram showing chlorine adducts consistently formed when Bond Elut PPL cartridges were washed with HCl water prior to elution. These data are from previous work, including sampling at multiple lakes and streams in Sweden, and motivates the choice of washing solvent (0.1% formic acid water) in this study.

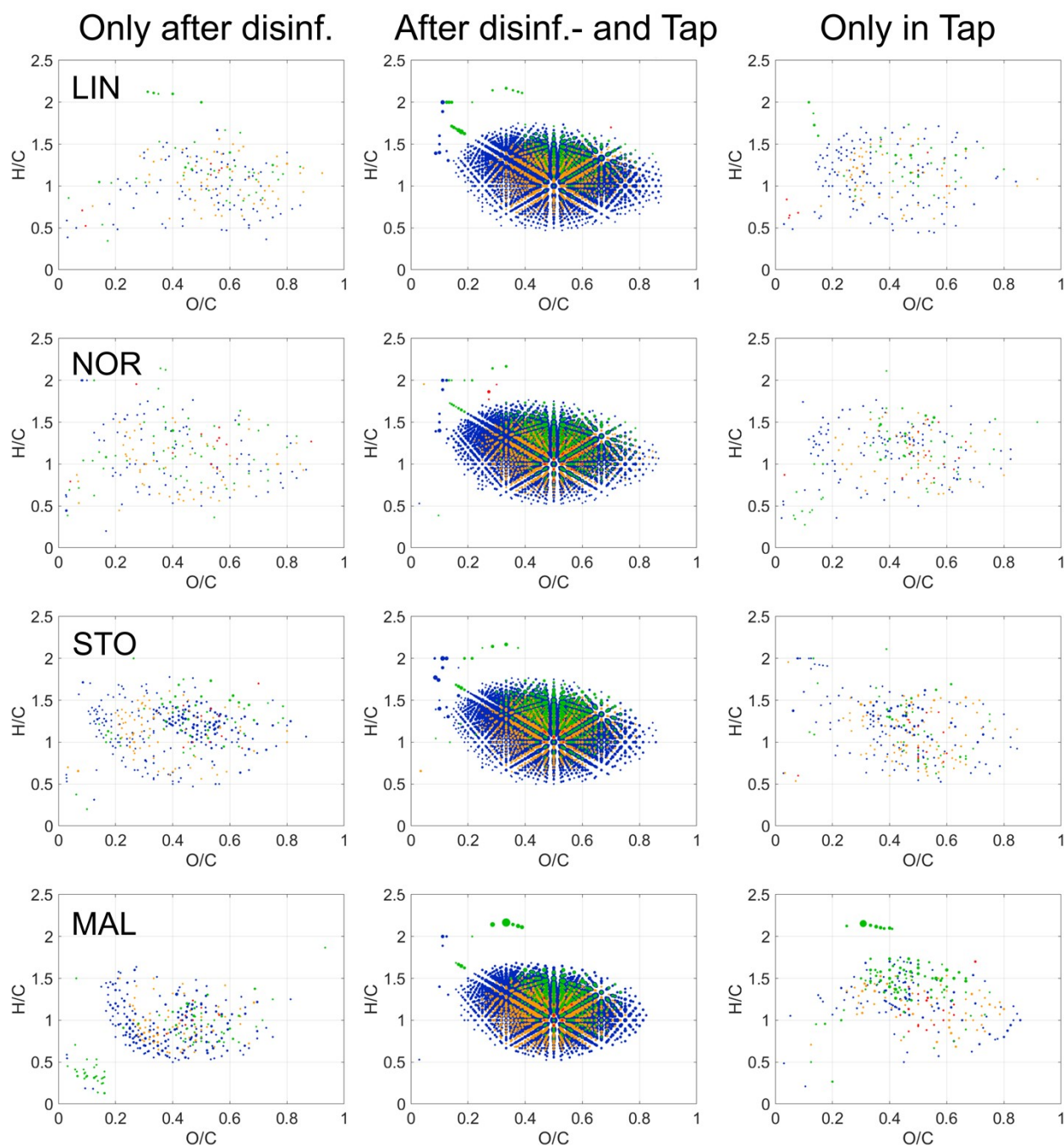


**Figure S10.** Relative contribution of CHO-, CHNO- and CHOS-type halogenated DOM molecular compositions detected throughout the treatment processes at LIN, NOR, STO and MAL (data from all five sampling occasions combined).

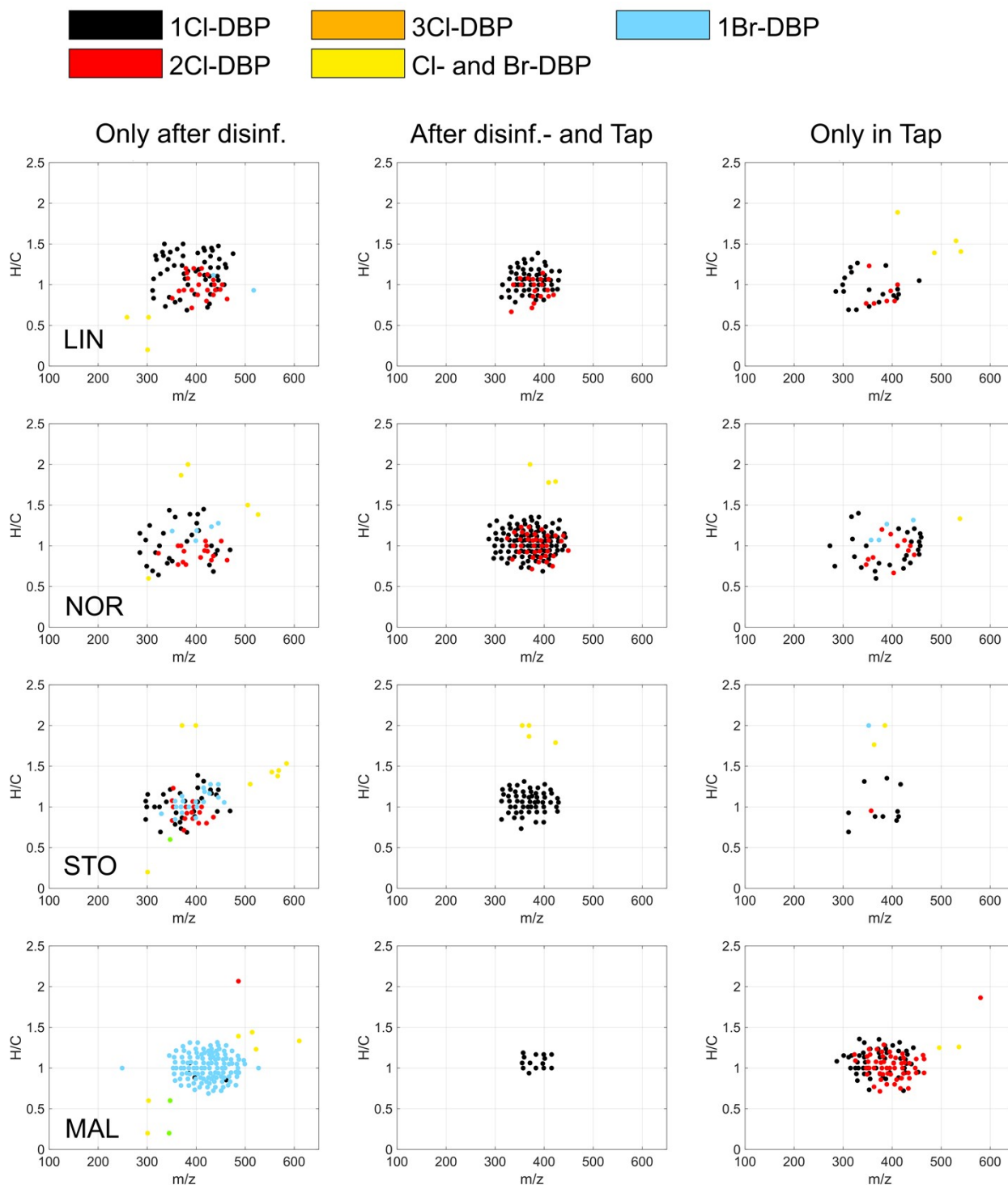


**Figure S11.** Overall distribution of the DOM molecular series, CHO, CHNO and CHOS of the chlorine- and bromine-containing DOM formulae including all sampling points (source water to tap) and consolidated formulae from all five sampling occasions.

■ CHO   
 ■ CHNO   
 ■ CHOS   
 ■ CHNOS



**Figure S12.** Van Krevelen plots for DOM molecular formulae detected only after chemical disinfection (left panel), at disinfection and in tap waters (middle panel) and in the tap waters only (right panel) at the four DWTPs (DBPs formed throughout the five sampling events combined). Note that Tap water at MAL is a mix of water from three DWTPs and therefore not directly comparable to the MAL DWTP water.



**Figure S13.** Edited H/C to mass plots for the verified DBPs detected after chemical disinfection only (left panel), at chemical disinfection and in tap waters (middle panel) and in the tap waters only (right panel) at the four DWTPs (DBPs formed throughout the five sampling events combined). Note that Tap water at MAL is a mix of water from three DWTPs and therefore not directly comparable to the MAL DWTP water.

**Table S1.** Raw water characteristics in LIN, NOR, STO and MAL. The average concentration of two replicates is reported for total nitrogen (TN), with standard deviation <0.01 mg L<sup>-1</sup> (LIN, NOR, STO) and <0.03 mg L<sup>-1</sup> (MAL). NR = Not reported.

<i>DWTP</i>	<i>Month</i>	<i>Temp</i>	<i>pH</i>	<i>Cond.</i>	<i>TN</i>	<i>DOC</i>	<i>UVA<sub>254</sub></i>	<i>SUVA</i>
		°C		µS cm <sup>-1</sup>	mg L <sup>-1</sup>	mg L <sup>-1</sup>	cm <sup>-1</sup>	L mg <sup>-1</sup> m <sup>-1</sup>
<i>LIN</i>	Mar	5.0	7.7	153	0.82	2.2	0.043	2.0
	May	12.4	7.7	154	0.63	2.8	0.043	1.6
	Aug	23.2	7.9	145	0.40	3.0	0.046	1.5
	Nov	3.3	7.6	149	0.47	2.8	0.039	1.4
	Jan	1.2	7.6	150	0.59	2.4	0.037	1.5
<i>NOR</i>	Mar	1.8	7.6	176	0.69	6.4	0.244	3.8
	May	10.9	7.6	178	0.77	5.6	0.221	3.9
	Aug	17.1	7.6	189	0.49	7.0	0.171	2.4
	Nov	5.8	7.8	195	0.48	6.4	0.168	2.6
	Jan	1.9	7.7	201	0.51	6.0	0.159	2.7
<i>STO</i>	Mar	5.0	7.8	225	0.66	7.5	0.231	3.1
	May	6.9	8.0	216	0.57	7.8	0.222	2.9
	Aug	11.1	7.4	210	0.59	7.9	0.213	2.7
	Nov	9.0	7.8	200	0.55	7.3	0.198	2.7
	Jan	1.8	7.8	203	0.55	7.0	0.195	2.8
<i>MAL</i>	Mar	9.0	7.4	719	1.30	2.6	NR	NR
	May	10.1	7.3	720	1.43	2.7	NR	NR
	Aug	10.2	7.3	718	1.39	2.6	NR	NR
	Nov	9.3	7.3	741	1.46	2.9	NR	NR
	Jan	8.8	7.2	747	1.63	2.4	NR	NR

**Table S2.** Counts of  $m/z$  ions and computed weighted indices of molecular formulae detected in the source water of LIN, NOR, STO and MAL throughout five sample occasions combined as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added).

Number of DOM compositions	LIN	NOR	STO	MAL
Total	10398	12642	10379	10521
CHO	7326	8775	7746	7214
CHNO	2245	2476	1698	2318
CHOS	802	1341	931	940
CHONS	25	50	4	49
Characteristics of CHO compositions				
average H [%]	45.2	43.5	43.7	44.6
average C [%]	36.9	37.7	37.6	37.8
average O [%]	18.0	18.8	18.7	17.5
computed average H/C ratio	1.23	1.15	1.16	1.18
computed average O/C ratio	0.49	0.50	0.50	0.46
average carbon oxidation state ( $C_{OS}$ )	-0.24	-0.14	-0.15	-0.24
average DBE	8.1	9.0	9.0	9.0
average DBE/C	0.44	0.48	0.47	0.46
average $AI_{mod}$	0.26	0.30	0.29	0.30
mass weighted average [Da]	386.9	397.6	406.8	403.4
Characteristics of CHNO compositions				
average H [%]	42.8	40.8	41.1	42.1
average C [%]	37.0	38.1	37.8	38.3
average O [%]	18.0	19.0	19.0	17.5
average N [%]	2.1	2.1	2.1	2.1
computed average H/C ratio	1.16	1.07	1.09	1.10
computed average O/C ratio	0.49	0.50	0.50	0.46
computed average N/C ratio	0.06	0.06	0.06	0.05
average carbon oxidation state ( $C_{OS}$ )	-0.18	-0.07	-0.08	-0.18
average DBE	8.9	9.8	9.7	9.9
average DBE/C	0.51	0.55	0.54	0.53
average $AI_{mod}$	0.31	0.36	0.35	0.35
mass weighted average [Da]	380.5	390.2	391.7	395.0
Characteristics of CHOS compositions				
average H [%]	46.4	44.5	46.3	43.8
average C [%]	33.9	34.8	34.1	36.0
average O [%]	17.6	18.6	17.5	18.1
average S [%]	2.1	2.1	2.1	2.1
computed average H/C ratio	1.37	1.28	1.36	1.21
computed average O/C ratio	0.52	0.53	0.51	0.50
computed average S/C ratio	0.06	0.06	0.06	0.06
average carbon oxidation state ( $C_{OS}$ )	-0.32	-0.20	-0.33	-0.21
average DBE	6.1	7.0	6.3	7.7
average DBE/C	0.38	0.42	0.38	0.45
average $AI_{mod}$	0.16	0.21	0.17	0.27
mass weighted average [Da]	383.7	394.6	386.9	393.3



**Table S3.** Water characteristics in LIN, NOR, STO and MAL at the point right before chemical disinfection. The average concentration of two replicates is reported for total nitrogen (TN), with standard deviation <0.01 mg L<sup>-1</sup> (LIN, NOR, STO) and <0.04 mg L<sup>-1</sup> (MAL).

<i>DWTP</i>	<i>Month</i>	<i>Temp</i>	<i>pH</i>	<i>Cond.</i>	<i>TN</i>	<i>DOC</i>	<i>UVA<sub>254</sub></i>	<i>SUVA</i>
		°C		µS cm <sup>-1</sup>	mg L <sup>-1</sup>	mg L <sup>-1</sup>	cm <sup>-1</sup>	L mg <sup>-1</sup> m <sup>-1</sup>
<i>LIN</i>	Mar	3.4	7.7	158	0.81	1.7	0.036	2.1
	May	13.6	7.4	159	0.59	2.0	0.029	1.5
	Aug	22.4	7.3	151	0.36	1.6	0.026	1.6
	Nov	3.8	7.4	150	0.44	2.2	0.029	1.3
	Jan	1.1	7.5	153	0.56	1.9	0.030	1.6
<i>NOR</i>	Mar	5.1	7.1	223	0.49	2.3	0.049	2.1
	May	12.8	7.2	224	0.63	2.9	0.048	1.7
	Aug	18.3	7.1	236	0.32	2.9	0.041	1.4
	Nov	6.1	7.1	236	0.33	2.9	0.044	1.5
	Jan	1.5	7.1	240	0.36	2.8	0.043	1.5
<i>STO</i>	Mar	5.4	7.0	244	0.52	4.3	0.083	1.9
	May	7.3	6.9	233	0.42	4.2	0.077	1.8
	Aug	10.7	6.8	222	0.46	4.6	0.079	1.7
	Nov	8.5	6.8	211	0.41	4.2	0.076	1.8
	Jan	2.0	6.9	213	0.43	4.1	0.079	1.9
<i>MAL</i>	Mar	9.1	8.1	373	1.25	2.4	0.057	2.4
	May	10.4	8.0	388	1.27	2.3	0.058	2.5
	Aug	10.6	8.2	365	1.19	2.3	0.057	2.5
	Nov	9.6	8.1	381	1.21	2.4	0.053	2.2
	Jan	8.7	8.0	383	1.43	2.2	0.051	2.3

**Table S4.** Counts of  $m/z$  ions and computed weighted indices of molecular formulae detected at the point right before chemical disinfection at LIN, NOR, STO and MAL throughout five sample occasions combined as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added).

Number of DOM compositions	LIN	NOR	STO	MAL
Total	10016	12652	9889	10882
CHO	6981	8008	7082	7130
CHNO	2159	2760	1693	2568
CHOS	851	1683	1065	1089
CHONS	25	201	49	95
Characteristics of CHO compositions				
average H [%]	44.6	45.6	45.5	44.2
average C [%]	36.9	37.1	37.1	37.8
average O [%]	18.5	17.3	17.4	18.0
computed average H/C ratio	1.21	1.23	1.23	1.17
computed average O/C ratio	0.50	0.47	0.47	0.48
average carbon oxidation state ( $C_{OS}$ )	-0.19	-0.28	-0.27	-0.21
average DBE	8.3	8.3	8.5	9.1
average DBE/C	0.45	0.44	0.44	0.47
average $AI_{mod}$	0.26	0.27	0.27	0.30
mass weighted average [Da]	393.4	391.3	402.3	405.5
Characteristics of CHNO compositions				
average H [%]	42.4	42.8	42.7	41.4
average C [%]	37.1	37.4	37.5	38.5
average O [%]	18.5	17.6	17.8	18.0
average N [%]	2.1	2.1	2.1	2.1
computed average H/C ratio	1.14	1.14	1.14	1.08
computed average O/C ratio	0.50	0.47	0.47	0.47
computed average N/C ratio	0.057	0.055	0.055	0.053
average carbon oxidation state ( $C_{OS}$ )	-0.14	-0.19	-0.18	-0.14
average DBE	9.1	9.2	9.3	10.1
average DBE/C	0.51	0.51	0.51	0.54
average $AI_{mod}$	0.34	0.35	0.35	0.39
mass weighted average [Da]	387.9	387.6	392.3	399.6
Characteristics of CHOS compositions				
average H [%]	45.8	45.0	46.2	43.5
average C [%]	33.9	34.9	34.5	35.9
average O [%]	18.2	18.0	17.3	18.5
average S [%]	2.1	2.1	2.0	2.1
computed average H/C ratio	1.35	1.29	1.34	1.21
computed average O/C ratio	0.54	0.52	0.50	0.51
computed average S/C ratio	0.061	0.060	0.059	0.059
average carbon oxidation state ( $C_{OS}$ )	-0.27	-0.25	-0.33	-0.18
average DBE	6.3	6.9	6.6	7.7
average DBE/C	0.39	0.42	0.39	0.45
average $AI_{mod}$	0.08	0.14	0.11	0.20
mass weighted average [Da]	391.5	391.7	392.4	394.8

**Table S5.** Counts of  $m/z$  ions and computed weighted indices of molecular formulae, focused on DOM, detected at the point right after chemical disinfection at LIN, NOR, STO and MAL throughout five sample occasions combined as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added).

Number of DOM compositions	LIN	NOR	STO	MAL
Total	9806	11961	9794	10046
CHO	6788	7689	6967	6727
CHNO	2193	2706	1679	2356
CHOS	816	1463	1120	938
CHONS	9	103	28	25
<b>Characteristics of CHO compositions</b>				
average H [%]	44.4	45.7	45.5	44.4
average C [%]	36.9	37.1	37.1	37.6
average O [%]	18.7	17.2	17.4	18.0
computed average H/C ratio	1.21	1.23	1.23	1.18
computed average O/C ratio	0.51	0.46	0.47	0.48
average carbon oxidation state ( $C_{OS}$ )	-0.18	-0.29	-0.27	-0.21
average DBE	8.3	8.2	8.5	9.0
average DBE/C	0.45	0.44	0.44	0.46
average $AI_{mod}$	0.26	0.27	0.27	0.29
mass weighted average [Da]	390.9	387.6	400.5	403.8
<b>Characteristics of CHNO compositions</b>				
average H [%]	42.1	42.7	42.7	41.6
average C [%]	36.9	37.4	37.3	38.1
average O [%]	18.9	17.8	17.9	18.2
average N [%]	2.1	2.1	2.1	2.1
computed average H/C ratio	1.14	1.14	1.14	1.09
computed average O/C ratio	0.51	0.48	0.48	0.48
computed average N/C ratio	0.06	0.06	0.06	0.05
average carbon oxidation state ( $C_{OS}$ )	-0.11	-0.18	-0.18	-0.13
average DBE	9.0	9.1	9.2	9.9
average DBE/C	0.52	0.51	0.51	0.54
average $AI_{mod}$	0.33	0.35	0.34	0.38
mass weighted average [Da]	385.8	383.0	389.9	396.9
<b>Characteristics of CHOS compositions</b>				
average H [%]	46.6	45.5	46.4	44.1
average C [%]	33.6	34.6	34.3	35.8
average O [%]	17.8	17.9	17.3	18.1
average S [%]	2.1	2.1	2.0	2.1
computed average H/C ratio	1.39	1.32	1.35	1.23
computed average O/C ratio	0.53	0.52	0.50	0.51
computed average S/C ratio	0.06	0.06	0.06	0.06
average carbon oxidation state ( $C_{OS}$ )	-0.32	-0.27	-0.34	-0.23
average DBE	6.0	6.7	6.5	7.6
average DBE/C	0.37	0.40	0.38	0.44
average $AI_{mod}$	0.06	0.12	0.10	0.17
mass weighted average [Da]	389.3	390.6	394.0	396.2

**Table S6.** Counts of  $m/z$  ions and computed weighted indices of molecular formulae, focused on DOM, detected in the tap waters at LIN, NOR, STO and MAL throughout five sample occasions combined as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added).

Number of DOM compositions	LIN	NOR	STO	MAL
Total	10097	11813	10569	9718
CHO	7068	7659	7438	6334
CHNO	2226	2657	1955	2330
CHOS	793	1403	1140	1012
CHONS	10	94	36	42
Characteristics of CHO compositions				
average H [%]	44.7	45.8	45.7	44.8
average C [%]	36.9	37.1	37.1	37.4
average O [%]	18.4	17.2	17.2	17.8
computed average H/C ratio	1.21	1.23	1.23	1.20
computed average O/C ratio	0.50	0.46	0.46	0.48
average carbon oxidation state ( $C_{OS}$ )	-0.20	-0.29	-0.29	-0.23
average DBE	8.2	8.2	8.4	8.7
average DBE/C	0.45	0.44	0.44	0.45
average $AI_{mod}$	0.27	0.26	0.27	0.28
mass weighted average [Da]	387.2	389.4	399.3	397.4
Characteristics of CHNO compositions				
average H [%]	42.3	42.9	42.7	42.0
average C [%]	37.0	37.3	37.4	37.7
average O [%]	18.5	17.7	17.9	18.2
average N [%]	2.1	2.1	2.1	2.1
computed average H/C ratio	1.14	1.15	1.14	1.11
computed average O/C ratio	0.50	0.48	0.48	0.48
computed average N/C ratio	0.06	0.06	0.06	0.05
average carbon oxidation state ( $C_{OS}$ )	-0.14	-0.19	-0.18	-0.14
average DBE	8.9	9.1	9.3	9.6
average DBE/C	0.52	0.51	0.51	0.53
average $AI_{mod}$	0.34	0.34	0.34	0.36
mass weighted average [Da]	380.5	385.6	391.2	394.9
Characteristics of CHOS compositions				
average H [%]	46.2	45.4	46.4	46.8
average C [%]	33.7	34.6	34.3	34.1
average O [%]	18.0	17.9	17.3	17.1
average S [%]	2.1	2.1	2.0	2.0
computed average H/C ratio	1.37	1.31	1.35	1.38
computed average O/C ratio	0.53	0.52	0.50	0.50
computed average S/C ratio	0.06	0.06	0.06	0.06
average carbon oxidation state ( $C_{OS}$ )	-0.30	-0.27	-0.34	-0.38
average DBE	6.1	6.7	6.5	6.2
average DBE/C	0.38	0.40	0.38	0.37
average $AI_{mod}$	0.07	0.12	0.10	0.08
mass weighted average [Da]	389.3	392.0	391.2	390.6

**Table S7.** Counts of  $m/z$  ions and computed weighted indices of DBP molecular formulae detected both after disinfection and in tap water (left column) and those solely detected in tap waters (right column) of LIN, NOR, STO and MAL throughout five sampling occasions as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added).

DBP characteristics	LIN		NOR		STO		MAL	
	DWTP +Tap	Tap only	DWTP +Tap	Tap only	DWTP +Tap	Tap only	DWTP +Tap	Tap only
number of DBP compositions	74	30	145	42	59	14	14	110
average H [%]	38.9	40.7	39.9	39.1	44.5	47.4	41.2	40.2
average C [%]	37.6	38.3	37.8	38.2	37.0	36.9	38.2	37.5
average O [%]	20.7	17.6	19.5	19.8	15.9	12.6	18.3	18.9
average N [%]	0	0.16	0	0.03	0	0.14	0	0.05
average S [%]	0	0.05	0.01	0.00	0.02	0	0	0.02
average Cl [%]	2.8	2.9	2.8	2.7	2.3	2.2	2.3	3.3
average Br [%]	0	0.2	0.03	0.1	0.3	0.7	0	0.04
computed average H/C ratio	1.04	1.06	1.06	1.02	1.20	1.28	1.08	1.07
computed average O/C ratio	0.55	0.46	0.51	0.52	0.43	0.34	0.48	0.50
average carbon oxidation state ( $C_{OS}$ )	0.15	0.01	0.06	0.12	-0.27	-0.53	-0.06	0.06
average DBE	7.8	7.9	7.8	8.5	6.8	6.4	8.1	7.7
average DBE/C	0.51	0.49	0.50	0.51	0.43	0.38	0.49	0.48
average $AI_{mod}$	0.38	0.40	0.38	0.39	0.32	0.30	0.37	0.37
mass weighted average [Da]	372.5	379.9	372.8	403.1	369.0	378.2	377.8	386.7

**Table S8.** List of verified DBP molecular compositions detected both after chemical disinfection and in tap water at the four DWTPs, LIN, NOR, STO and MAL, including data for all five sampling occasions. Note that each DBP formula is reported once for each DWTP, even though they were detected at multiple sampling occasions.

DWTP	DBP Formula Neutral form	Theoretical Mass Negative Ion
LIN	C12 H12 O7 Cl2	336.98874
LIN	C12 H12 O8 Cl2	352.98365
LIN	C12 H8 O7 Cl2	332.95744
LIN	C13 H10 O9 Cl2	378.96292
LIN	C13 H11 O7 Cl1	313.01206
LIN	C13 H11 O8 Cl1	329.00697
LIN	C13 H12 O9 Cl2	380.97857
LIN	C13 H13 O7 Cl1	315.02771
LIN	C13 H13 O9 Cl1	347.01754
LIN	C13 H14 O7 Cl2	351.00439
LIN	C13 H14 O8 Cl2	366.9993
LIN	C13 H15 O8 Cl1	333.03827
LIN	C14 H10 O8 Cl2	374.968
LIN	C14 H11 O8 Cl1	341.00697
LIN	C14 H12 O10 Cl2	408.97348
LIN	C14 H12 O8 Cl2	376.98365
LIN	C14 H12 O9 Cl2	392.97857
LIN	C14 H13 O7 Cl1	327.02771
LIN	C14 H13 O8 Cl1	343.02262
LIN	C14 H13 O9 Cl1	359.01754
LIN	C14 H14 O8 Cl2	378.9993
LIN	C14 H14 O9 Cl2	394.99422
LIN	C14 H15 O7 Cl1	329.04336
LIN	C14 H15 O8 Cl1	345.03827
LIN	C14 H15 O9 Cl1	361.03319
LIN	C14 H16 O9 Cl2	397.00987
LIN	C14 H17 O7 Cl1	331.05901
LIN	C14 H17 O8 Cl1	347.05392
LIN	C15 H13 O10 Cl1	387.01245
LIN	C15 H13 O8 Cl1	355.02262
LIN	C15 H13 O9 Cl1	371.01754
LIN	C15 H14 O9 Cl2	406.99422
LIN	C15 H15 O10 Cl1	389.0281
LIN	C15 H15 O7 Cl1	341.04336
LIN	C15 H15 O8 Cl1	357.03827
LIN	C15 H15 O9 Cl1	373.03319
LIN	C15 H16 O7 Cl2	377.02004
LIN	C15 H16 O8 Cl2	393.01495
LIN	C15 H16 O9 Cl2	409.00987
LIN	C15 H17 O10 Cl1	391.04375

LIN	C15 H17 O7 Cl1	343.05901
LIN	C15 H17 O8 Cl1	359.05392
LIN	C15 H19 O7 Cl1	345.07466
LIN	C15 H19 O8 Cl1	361.06957
LIN	C16 H13 O10 Cl1	399.01245
LIN	C16 H13 O9 Cl1	383.01754
LIN	C16 H14 O9 Cl2	418.99422
LIN	C16 H15 O10 Cl1	401.0281
LIN	C16 H15 O11 Cl1	417.02302
LIN	C16 H15 O8 Cl1	369.03827
LIN	C16 H15 O9 Cl1	385.03319
LIN	C16 H17 O10 Cl1	403.04375
LIN	C16 H17 O7 Cl1	355.05901
LIN	C16 H17 O8 Cl1	371.05392
LIN	C16 H17 O9 Cl1	387.04884
LIN	C16 H19 O7 Cl1	357.07466
LIN	C16 H19 O8 Cl1	373.06957
LIN	C16 H19 O9 Cl1	389.06449
LIN	C16 H21 O7 Cl1	359.09031
LIN	C16 H21 O8 Cl1	375.08522
LIN	C17 H17 O10 Cl1	415.04375
LIN	C17 H17 O9 Cl1	399.04884
LIN	C17 H19 O7 Cl1	369.07466
LIN	C17 H19 O8 Cl1	385.06957
LIN	C17 H19 O9 Cl1	401.06449
LIN	C17 H21 O9 Cl1	403.08014
LIN	C18 H17 O10 Cl1	427.04375
LIN	C18 H19 O10 Cl1	429.0594
LIN	C18 H19 O8 Cl1	397.06957
LIN	C18 H19 O9 Cl1	413.06449
LIN	C18 H21 O10 Cl1	431.07505
LIN	C18 H21 O9 Cl1	415.08014
LIN	C18 H23 O8 Cl1	401.10087
LIN	C18 H25 O7 Cl1	387.12161
NOR	C11 H12 O7 Cl2	324.98874
NOR	C12 H10 O7 Cl2	334.97309
NOR	C12 H11 O7 Cl1	301.01206
NOR	C12 H12 O7 Cl2	336.98874
NOR	C12 H12 O8 Cl2	352.98365
NOR	C12 H13 O6 Cl1	287.03279
NOR	C12 H13 O7 Cl1	303.02771
NOR	C12 H14 O7 Cl2	339.00439
NOR	C12 H14 O8 Cl2	354.9993
NOR	C12 H15 O6 Cl1	289.04844
NOR	C13 H11 O6 Cl1	297.01714
NOR	C13 H11 O7 Cl1	313.01206
NOR	C13 H11 O8 Cl1	329.00697
NOR	C13 H12 O7 Cl2	348.98874

NOR	C13 H12 O8 CI2	364.98365
NOR	C13 H12 O9 CI2	380.97857
NOR	C13 H13 O6 CI1	299.03279
NOR	C13 H13 O7 CI1	315.02771
NOR	C13 H13 O8 CI1	331.02262
NOR	C13 H14 O7 CI2	351.00439
NOR	C13 H14 O8 CI2	366.9993
NOR	C13 H14 O9 CI2	382.99422
NOR	C13 H15 O6 CI1	301.04844
NOR	C13 H15 O7 CI1	317.04336
NOR	C13 H16 O7 CI2	353.02004
NOR	C13 H16 O8 CI2	369.01495
NOR	C13 H17 O6 CI1	303.06409
NOR	C14 H10 O8 CI2	374.968
NOR	C14 H11 O7 CI1	325.01206
NOR	C14 H11 O9 CI1	357.00189
NOR	C14 H12 O8 CI2	376.98365
NOR	C14 H12 O9 CI2	392.97857
NOR	C14 H13 O10 CI1	375.01245
NOR	C14 H13 O6 CI1	311.03279
NOR	C14 H13 O7 CI1	327.02771
NOR	C14 H13 O8 CI1	343.02262
NOR	C14 H13 O9 CI1	359.01754
NOR	C14 H14 O8 CI2	378.9993
NOR	C14 H14 O9 CI2	394.99422
NOR	C14 H15 O6 CI1	313.04844
NOR	C14 H15 O7 CI1	329.04336
NOR	C14 H15 O8 CI1	345.03827
NOR	C14 H15 O9 CI1	361.03319
NOR	C14 H16 O7 CI2	365.02004
NOR	C14 H16 O8 CI2	381.01495
NOR	C14 H17 O6 CI1	315.06409
NOR	C14 H17 O7 CI1	331.05901
NOR	C14 H17 O8 CI1	347.05392
NOR	C14 H19 O7 CI1	333.07466
NOR	C15 H11 O8 CI1	353.00697
NOR	C15 H11 O9 CI1	369.00189
NOR	C15 H12 O8 CI2	388.98365
NOR	C15 H12 O9 CI2	404.97857
NOR	C15 H13 O10 CI1	387.01245
NOR	C15 H13 O7 CI1	339.02771
NOR	C15 H13 O8 CI1	355.02262
NOR	C15 H13 O9 CI1	371.01754
NOR	C15 H14 O8 CI2	390.9993
NOR	C15 H14 O9 CI2	406.99422
NOR	C15 H15 O10 CI1	389.0281
NOR	C15 H15 O7 CI1	341.04336
NOR	C15 H15 O8 CI1	357.03827



NOR	C15 H15 O9 CI1	373.03319
NOR	C15 H16 O7 CI2	377.02004
NOR	C15 H16 O8 CI2	393.01495
NOR	C15 H16 O9 CI2	409.00987
NOR	C15 H17 O6 CI1	327.06409
NOR	C15 H17 O7 CI1	343.05901
NOR	C15 H17 O8 CI1	359.05392
NOR	C15 H17 O9 CI1	375.04884
NOR	C15 H18 O8 CI2	395.0306
NOR	C15 H19 O6 CI1	329.07974
NOR	C15 H19 O7 CI1	345.07466
NOR	C15 H19 O8 CI1	361.06957
NOR	C15 H30 O3 CI1 Br1	371.09941
NOR	C16 H11 O10 CI1	396.9968
NOR	C16 H12 O9 CI2	416.97857
NOR	C16 H13 O10 CI1	399.01245
NOR	C16 H13 O8 CI1	367.02262
NOR	C16 H13 O9 CI1	383.01754
NOR	C16 H14 O8 CI2	402.9993
NOR	C16 H14 O9 CI2	418.99422
NOR	C16 H15 O10 CI1	401.0281
NOR	C16 H15 O7 CI1	353.04336
NOR	C16 H15 O8 CI1	369.03827
NOR	C16 H15 O9 CI1	385.03319
NOR	C16 H16 O8 CI2	405.01495
NOR	C16 H17 O10 CI1	403.04375
NOR	C16 H17 O6 CI1	339.06409
NOR	C16 H17 O7 CI1	355.05901
NOR	C16 H17 O8 CI1	371.05392
NOR	C16 H17 O9 CI1	387.04884
NOR	C16 H18 O10 CI2	439.02043
NOR	C16 H18 O8 CI2	407.0306
NOR	C16 H18 O9 CI2	423.02552
NOR	C16 H19 O6 CI1	341.07974
NOR	C16 H19 O7 CI1	357.07466
NOR	C16 H19 O8 CI1	373.06957
NOR	C16 H19 O9 CI1	389.06449
NOR	C16 H21 O7 CI1	359.09031
NOR	C16 H21 O8 CI1	375.08522
NOR	C17 H13 O10 CI1	411.01245
NOR	C17 H15 O10 CI1	413.0281
NOR	C17 H15 O8 CI1	381.03827
NOR	C17 H15 O9 CI1	397.03319
NOR	C17 H16 O10 CI2	449.00478
NOR	C17 H17 O10 CI1	415.04375
NOR	C17 H17 O7 CI1	367.05901
NOR	C17 H17 O8 CI1	383.05392
NOR	C17 H17 O9 CI1	399.04884

NOR	C17 H18 O9 Cl2	435.02552
NOR	C17 H19 O10 Cl1	417.0594
NOR	C17 H19 O6 Cl1	353.07974
NOR	C17 H19 O7 Cl1	369.07466
NOR	C17 H19 O8 Cl1	385.06957
NOR	C17 H19 O9 Cl1	401.06449
NOR	C17 H21 O7 Cl1	371.09031
NOR	C17 H21 O8 Cl1	387.08522
NOR	C17 H21 O9 Cl1	403.08014
NOR	C17 H23 O7 Cl1	373.10596
NOR	C17 H23 O8 Cl1	389.10087
NOR	C18 H15 O9 Cl1	409.03319
NOR	C18 H17 O10 Cl1	427.04375
NOR	C18 H17 O8 Cl1	395.05392
NOR	C18 H17 O9 Cl1	411.04884
NOR	C18 H19 O10 Cl1	429.0594
NOR	C18 H19 O8 Cl1	397.06957
NOR	C18 H19 O9 Cl1	413.06449
NOR	C18 H21 O7 Cl1	383.09031
NOR	C18 H21 O8 Cl1	399.08522
NOR	C18 H21 O9 Cl1	415.08014
NOR	C18 H23 O7 Cl1	385.10596
NOR	C18 H23 O9 Cl1	417.09579
NOR	C18 H32 O1 S1 Cl1 Br1	409.0973
NOR	C19 H17 O9 Cl1	423.04884
NOR	C19 H19 O10 Cl1	441.0594
NOR	C19 H19 O9 Cl1	425.06449
NOR	C19 H21 O10 Cl1	443.07505
NOR	C19 H21 O8 Cl1	411.08522
NOR	C19 H21 O9 Cl1	427.08014
NOR	C19 H23 O9 Cl1	429.09579
NOR	C19 H25 O9 Cl1	431.11144
NOR	C19 H34 O1 S1 Cl1 Br1	423.11295
NOR	C20 H19 O9 Cl1	437.06449
NOR	C20 H23 O9 Cl1	441.09579
STO	C13 H11 O7 Cl1	313.01206
STO	C13 H13 O8 Cl1	331.02262
STO	C13 H15 O7 Cl1	317.04336
STO	C14 H13 O7 Cl1	327.02771
STO	C14 H13 O8 Cl1	343.02262
STO	C14 H15 O6 Cl1	313.04844
STO	C14 H15 O7 Cl1	329.04336
STO	C14 H15 O8 Cl1	345.03827
STO	C14 H17 O6 Cl1	315.06409
STO	C14 H17 O7 Cl1	331.05901
STO	C15 H11 O8 Cl1	353.00697
STO	C15 H13 O7 Cl1	339.02771
STO	C15 H13 O8 Cl1	355.02262

STO	C15 H15 O7 CI1	341.04336
STO	C15 H15 O8 CI1	357.03827
STO	C15 H15 O9 CI1	373.03319
STO	C15 H17 O6 CI1	327.06409
STO	C15 H17 O7 CI1	343.05901
STO	C15 H17 O8 CI1	359.05392
STO	C15 H17 O9 CI1	375.04884
STO	C15 H19 O6 CI1	329.07974
STO	C15 H19 O7 CI1	345.07466
STO	C15 H28 O3 CI1 Br1	369.08376
STO	C15 H30 O2 CI1 Br1	355.1045
STO	C16 H13 O10 CI1	399.01245
STO	C16 H13 O9 CI1	383.01754
STO	C16 H15 O10 CI1	401.0281
STO	C16 H15 O7 CI1	353.04336
STO	C16 H15 O8 CI1	369.03827
STO	C16 H15 O9 CI1	385.03319
STO	C16 H17 O7 CI1	355.05901
STO	C16 H17 O8 CI1	371.05392
STO	C16 H17 O9 CI1	387.04884
STO	C16 H19 O6 CI1	341.07974
STO	C16 H19 O7 CI1	357.07466
STO	C16 H19 O8 CI1	373.06957
STO	C16 H21 O7 CI1	359.09031
STO	C16 H32 O2 CI1 Br1	369.12015
STO	C17 H17 O7 CI1	367.05901
STO	C17 H17 O8 CI1	383.05392
STO	C17 H17 O9 CI1	399.04884
STO	C17 H19 O7 CI1	369.07466
STO	C17 H19 O8 CI1	385.06957
STO	C17 H19 O9 CI1	401.06449
STO	C17 H21 O7 CI1	371.09031
STO	C17 H21 O8 CI1	387.08522
STO	C18 H17 O10 CI1	427.04375
STO	C18 H19 O10 CI1	429.0594
STO	C18 H19 O7 CI1	381.07466
STO	C18 H19 O8 CI1	397.06957
STO	C18 H19 O9 CI1	413.06449
STO	C18 H21 O7 CI1	383.09031
STO	C18 H21 O8 CI1	399.08522
STO	C18 H21 O9 CI1	415.08014
STO	C18 H23 O8 CI1	401.10087
STO	C19 H19 O9 CI1	425.06449
STO	C19 H21 O9 CI1	427.08014
STO	C19 H23 O8 CI1	413.10087
STO	C19 H34 O1 S1 CI1 Br1	423.11295
MAL	C15 H15 O8 CI1	357.03827
MAL	C15 H17 O8 CI1	359.05392

MAL	C16 H15 O8 Cl1	369.03827
MAL	C16 H17 O7 Cl1	355.05901
MAL	C16 H17 O8 Cl1	371.05392
MAL	C16 H19 O7 Cl1	357.07466
MAL	C17 H17 O10 Cl1	415.04375
MAL	C17 H17 O8 Cl1	383.05392
MAL	C17 H17 O9 Cl1	399.04884
MAL	C17 H19 O9 Cl1	401.06449
MAL	C18 H19 O8 Cl1	397.06957
MAL	C18 H21 O7 Cl1	383.09031
MAL	C18 H21 O8 Cl1	399.08522
MAL	C18 H21 O9 Cl1	415.08014

**Table S9.** List of verified DBP molecular compositions detected in tap water samples only, i.e., DBPs detected in tap waters but not right after chemical disinfection, from the four DWTPs, LIN, NOR, STO and MAL, including data for all five sampling occasions. Note that each DBP formula is reported once for each DWTP, even though they were detected at multiple sampling occasions.

<b>DWTP</b>	<b>DBP Formula Neutral form</b>	<b>Theoretical Mass Negative Ion</b>
LIN	C12 H11 O6 Cl1	285.01714
LIN	C12 H11 O7 Cl1	301.01206
LIN	C12 H13 O7 Cl1	303.02771
LIN	C13 H10 O7 Cl2	346.97309
LIN	C13 H10 O8 Cl2	362.968
LIN	C13 H12 O10 Cl2	396.97348
LIN	C13 H13 O6 Cl1	299.03279
LIN	C13 H15 O7 Cl1	317.04336
LIN	C13 H16 O7 Cl2	353.02004
LIN	C13 H9 O7 Cl1	310.99641
LIN	C13 H9 O8 Cl1	326.99132
LIN	C14 H11 O10 Cl1	372.9968
LIN	C14 H14 O10 Cl2	410.98913
LIN	C14 H17 O6 Cl1	315.06409
LIN	C15 H11 O8 Cl1	353.00697
LIN	C15 H12 O8 Cl2	388.98365
LIN	C15 H12 O9 Cl2	404.97857
LIN	C15 H13 O11 Cl1	403.00737
LIN	C15 H19 O6 Cl1	329.07974
LIN	C16 H15 O7 Cl1	353.04336
LIN	C17 H15 O10 Cl1	413.0281
LIN	C17 H15 O8 Cl1	381.03827
LIN	C17 H21 O8 Cl1	387.08522
LIN	C18 H15 O9 Cl1	409.03319
LIN	C18 H17 O9 Cl1	411.04884
LIN	C18 H34 O1 S1 Cl1 Br1	411.11295
LIN	C20 H21 O10 Cl1	455.07505
LIN	C23 H32 O1 N1 Cl2 Br1	486.09716
LIN	C26 H40 O1 N1 Cl2 Br1	530.15976
LIN	C27 H38 O1 N1 Cl2 Br1	540.14411
NOR	C11 H11 O6 Cl1	273.01714
NOR	C12 H10 O8 Cl2	350.968
NOR	C12 H13 O8 Cl1	319.02262
NOR	C12 H9 O6 Cl1	283.00149
NOR	C13 H10 O7 Cl2	346.97309
NOR	C13 H13 O9 Cl1	347.01754
NOR	C14 H11 O10 Cl1	372.9968
NOR	C14 H12 O7 Cl2	360.98874
NOR	C14 H14 O10 Cl2	410.98913
NOR	C14 H15 O6 Br1	356.99793

NOR	C14 H15 O7 Br1	372.99284
NOR	C14 H16 O9 Cl2	397.00987
NOR	C14 H19 O6 Cl1	317.07974
NOR	C15 H10 O9 Cl2	402.96292
NOR	C15 H11 O7 Cl1	337.01206
NOR	C15 H13 O6 Cl1	323.03279
NOR	C15 H16 O10 Cl2	425.00478
NOR	C15 H18 O7 Cl2	379.03569
NOR	C15 H19 O7 Br1	389.02414
NOR	C15 H21 O6 Cl1	331.09539
NOR	C15 H9 O9 Cl1	366.98624
NOR	C16 H11 O8 Cl1	365.00697
NOR	C16 H16 O10 Cl2	437.00478
NOR	C17 H13 O9 Cl1	395.01754
NOR	C17 H15 O11 Cl1	429.02302
NOR	C17 H16 O9 Cl2	433.00987
NOR	C18 H13 O10 Cl1	423.01245
NOR	C18 H15 O10 Cl1	425.0281
NOR	C18 H16 O9 Cl2	445.00987
NOR	C18 H21 O10 Cl1	431.07505
NOR	C19 H15 O10 Cl1	437.0281
NOR	C19 H17 O11 Cl1	455.03867
NOR	C19 H19 O11 Cl1	457.05432
NOR	C19 H21 O11 Cl1	459.06997
NOR	C19 H23 O10 Cl1	445.0907
NOR	C19 H23 O8 Cl1	413.10087
NOR	C19 H25 O7 Br1	443.07109
NOR	C20 H19 O10 Cl1	453.0594
NOR	C20 H21 O10 Cl1	455.07505
NOR	C20 H21 O9 Cl1	439.08014
NOR	C20 H23 O10 Cl1	457.0907
NOR	C27 H36 O1 N1 Cl2 Br1	538.12846
STO	C13 H9 O7 Cl1	310.99641
STO	C14 H13 O6 Cl1	311.03279
STO	C14 H28 O4 N1 Br1	352.1129
STO	C16 H21 O6 Cl1	343.09539
STO	C16 H32 O3 Cl1 Br1	385.11506
STO	C17 H15 O10 Cl1	413.0281
STO	C17 H15 O7 Cl1	365.04336
STO	C17 H15 O8 Cl1	381.03827
STO	C17 H23 O8 Cl1	389.10087
STO	C17 H30 O1 Cl1 Br1	363.10958
STO	C18 H15 O9 Cl1	409.03319
STO	C18 H17 O9 Cl1	411.04884
STO	C18 H23 O9 Cl1	417.09579
STO	C21 H20 O1 Cl2	357.08185
MAL	C11 H12 O7 Cl2	324.98874
MAL	C12 H12 O8 Cl2	352.98365

MAL	C12 H13 O6 Cl1	287.03279
MAL	C12 H14 O6 Cl2	323.00947
MAL	C12 H14 O8 Cl2	354.9993
MAL	C13 H10 O8 Cl2	362.968
MAL	C13 H11 O8 Cl1	329.00697
MAL	C13 H12 O10 Cl2	396.97348
MAL	C13 H12 O7 Cl2	348.98874
MAL	C13 H12 O9 Cl2	380.97857
MAL	C13 H13 O7 Cl1	315.02771
MAL	C13 H13 O8 Cl1	331.02262
MAL	C13 H13 O9 Cl1	347.01754
MAL	C13 H14 O7 Cl2	351.00439
MAL	C13 H14 O8 Cl2	366.9993
MAL	C13 H14 O9 Cl2	382.99422
MAL	C13 H15 O6 Cl1	301.04844
MAL	C13 H15 O7 Cl1	317.04336
MAL	C13 H15 O8 Cl1	333.03827
MAL	C13 H16 O7 Cl2	353.02004
MAL	C13 H16 O8 Cl2	369.01495
MAL	C14 H10 O8 Cl2	374.968
MAL	C14 H12 O10 Cl2	408.97348
MAL	C14 H12 O8 Cl2	376.98365
MAL	C14 H13 O10 Cl1	375.01245
MAL	C14 H13 O7 Cl1	327.02771
MAL	C14 H13 O8 Cl1	343.02262
MAL	C14 H14 O6 Cl2	347.00947
MAL	C14 H14 O7 Cl2	363.00439
MAL	C14 H14 O8 Cl2	378.9993
MAL	C14 H14 O9 Cl2	394.99422
MAL	C14 H15 O7 Cl1	329.04336
MAL	C14 H15 O8 Cl1	345.03827
MAL	C14 H16 O6 Cl2	349.02512
MAL	C14 H16 O8 Cl2	381.01495
MAL	C14 H16 O9 Cl2	397.00987
MAL	C14 H18 O8 Cl2	383.0306
MAL	C14 H19 O7 Cl1	333.07466
MAL	C15 H11 O8 Cl1	353.00697
MAL	C15 H12 O8 Cl2	388.98365
MAL	C15 H12 O9 Cl2	404.97857
MAL	C15 H13 O10 Cl1	387.01245
MAL	C15 H13 O8 Cl1	355.02262
MAL	C15 H14 O10 Cl2	422.98913
MAL	C15 H14 O7 Cl2	375.00439
MAL	C15 H14 O8 Cl2	390.9993
MAL	C15 H15 O6 Cl1	325.04844
MAL	C15 H15 O7 Cl1	341.04336
MAL	C15 H16 O10 Cl2	425.00478
MAL	C15 H16 O7 Cl2	377.02004

MAL	C15 H17 O5 CI1	311.06918
MAL	C15 H17 O7 CI1	343.05901
MAL	C15 H17 O9 CI1	375.04884
MAL	C15 H18 O7 CI2	379.03569
MAL	C15 H18 O8 CI2	395.0306
MAL	C16 H12 O10 CI2	432.97348
MAL	C16 H12 O9 CI2	416.97857
MAL	C16 H14 O10 CI2	434.98913
MAL	C16 H14 O9 CI2	418.99422
MAL	C16 H15 O7 CI1	353.04336
MAL	C16 H16 O7 CI2	389.02004
MAL	C16 H16 O8 CI2	405.01495
MAL	C16 H16 O9 CI2	421.00987
MAL	C16 H17 O10 CI1	403.04375
MAL	C16 H18 O8 CI2	407.0306
MAL	C16 H18 O9 CI2	423.02552
MAL	C16 H19 O6 CI1	341.07974
MAL	C16 H19 O8 CI1	373.06957
MAL	C16 H19 O9 CI1	389.06449
MAL	C16 H21 O6 CI1	343.09539
MAL	C17 H15 O10 CI1	413.0281
MAL	C17 H15 O8 CI1	381.03827
MAL	C17 H16 O10 CI2	449.00478
MAL	C17 H16 O11 CI2	464.9997
MAL	C17 H16 O9 CI2	433.00987
MAL	C17 H17 O6 CI1	351.06409
MAL	C17 H17 O7 CI1	367.05901
MAL	C17 H18 O7 CI2	403.03569
MAL	C17 H18 O8 CI2	419.0306
MAL	C17 H18 O9 CI2	435.02552
MAL	C17 H19 O10 CI1	417.0594
MAL	C17 H19 O8 CI1	385.06957
MAL	C17 H20 O8 CI2	421.04625
MAL	C17 H21 O6 CI1	355.09539
MAL	C17 H21 O7 CI1	371.09031
MAL	C17 H21 O8 CI1	387.08522
MAL	C17 H23 O7 CI1	373.10596
MAL	C18 H13 O10 CI1	423.01245
MAL	C18 H17 O10 CI1	427.04375
MAL	C18 H17 O8 CI1	395.05392
MAL	C18 H18 O9 CI2	447.02552
MAL	C18 H19 O10 CI1	429.0594
MAL	C18 H20 O10 CI2	465.03608
MAL	C18 H20 O9 CI2	449.04117
MAL	C18 H21 O10 CI1	431.07505
MAL	C18 H23 O7 CI1	385.10596
MAL	C18 H23 O8 CI1	401.10087
MAL	C19 H19 O9 CI1	425.06449



MAL	C19 H21 O9 Cl1	427.08014
MAL	C19 H22 O9 Cl2	463.05682
MAL	C19 H23 O8 Cl1	413.10087
MAL	C19 H23 O9 Cl1	429.09579
MAL	C19 H25 O8 Cl1	415.11652
MAL	C20 H19 O10 Cl1	453.0594
MAL	C20 H21 O9 Cl1	439.08014
MAL	C20 H25 O9 Cl1	443.11144
MAL	C22 H41 O10 N1 S1 Cl2	580.17555
MAL	C24 H30 O1 N1 Cl2 Br1	496.08151
MAL	C27 H34 O1 N1 Cl2 Br1	536.11281
MAL	C28 H49 O9 S1 Cl3	665.20901

**Table S10.** List of verified DBP molecular compositions detected after chemical disinfection only, i.e., DBPs detected in after chemical disinfection but not in tap waters, from the four DWTPs, LIN, NOR, STO and MAL, including data for all five sampling occasions. Note that each DBP formula is reported once for each DWTP, even though they were detected at multiple sampling occasions.

<b>DWTP</b>	<b>DBP Formula Neutral form</b>	<b>Theoretical Mass Negative Ion</b>
LIN	C12 H10 O8 Cl2	350.968
LIN	C13 H11 O9 Cl1	345.00189
LIN	C13 H12 O8 Cl2	364.98365
LIN	C13 H14 O9 Cl2	382.99422
LIN	C13 H17 O7 Cl1	319.05901
LIN	C14 H10 O9 Cl2	390.96292
LIN	C14 H11 O9 Cl1	357.00189
LIN	C14 H13 O6 Cl1	311.03279
LIN	C14 H15 O10 Cl1	377.0281
LIN	C14 H15 O6 Cl1	313.04844
LIN	C14 H16 O8 Cl2	381.01495
LIN	C14 H19 O6 Cl1	317.07974
LIN	C14 H19 O7 Cl1	333.07466
LIN	C14 H21 O7 Cl1	335.09031
LIN	C15 H11 O7 Cl1	337.01206
LIN	C15 H12 O10 Cl2	420.97348
LIN	C15 H14 O10 Cl2	422.98913
LIN	C15 H14 O11 Cl2	438.98405
LIN	C15 H14 O7 Cl2	375.00439
LIN	C15 H14 O8 Cl2	390.9993
LIN	C15 H17 O6 Cl1	327.06409
LIN	C15 H17 O9 Cl1	375.04884
LIN	C15 H18 O7 Cl2	379.03569
LIN	C15 H18 O8 Cl2	395.0306
LIN	C15 H18 O9 Cl2	411.02552
LIN	C15 H21 O6 Cl1	331.09539
LIN	C15 H21 O7 Cl1	347.09031
LIN	C16 H11 O9 Cl1	381.00189
LIN	C16 H13 O8 Cl1	367.02262
LIN	C16 H14 O10 Cl2	434.98913
LIN	C16 H14 O8 Cl2	402.9993
LIN	C16 H16 O10 Cl2	437.00478
LIN	C16 H16 O11 Cl2	452.9997
LIN	C16 H16 O8 Cl2	405.01495
LIN	C16 H17 O11 Cl1	419.03867
LIN	C16 H18 O8 Cl2	407.0306
LIN	C16 H18 O9 Cl2	423.02552
LIN	C16 H19 O10 Cl1	405.0594
LIN	C16 H19 O6 Cl1	341.07974
LIN	C16 H21 O6 Cl1	343.09539

LIN	C16 H23 O7 Cl1	361.10596
LIN	C17 H13 O11 Cl1	427.00737
LIN	C17 H14 O11 Cl2	462.98405
LIN	C17 H15 O11 Cl1	429.02302
LIN	C17 H15 O9 Cl1	397.03319
LIN	C17 H16 O10 Cl2	449.00478
LIN	C17 H17 O11 Cl1	431.03867
LIN	C17 H17 O8 Cl1	383.05392
LIN	C17 H18 O9 Cl2	435.02552
LIN	C17 H19 O10 Cl1	417.0594
LIN	C17 H21 O6 Cl1	355.09539
LIN	C17 H21 O7 Cl1	371.09031
LIN	C17 H23 O7 Cl1	373.10596
LIN	C18 H13 O10 Cl1	423.01245
LIN	C18 H15 O1 S1 Cl1	313.04594
LIN	C18 H17 O11 Cl1	443.03867
LIN	C18 H19 O11 Cl1	445.05432
LIN	C18 H21 O7 Cl1	383.09031
LIN	C18 H21 O8 Cl1	399.08522
LIN	C18 H23 O9 Cl1	417.09579
LIN	C18 H25 O8 Cl1	403.11652
LIN	C18 H27 O6 Cl1	373.14234
LIN	C19 H19 O11 Cl1	457.05432
LIN	C19 H21 O10 Cl1	443.07505
LIN	C19 H21 O9 Cl1	427.08014
LIN	C19 H23 O10 Cl1	445.0907
LIN	C19 H23 O11 Cl1	461.08562
LIN	C19 H23 O9 Cl1	429.09579
LIN	C19 H25 O10 Cl1	447.10635
LIN	C19 H27 O8 Cl1	417.13217
LIN	C19 H27 O9 Cl1	433.12709
LIN	C20 H25 O10 Cl1	459.10635
LIN	C20 H27 O8 Cl1	429.13217
LIN	C20 H29 O7 Cl1	415.15291
LIN	C20 H29 O8 Cl1	431.14782
LIN	C21 H29 O10 Cl1	475.13765
LIN	C21 H31 O8 Cl1	445.16347
LIN	C26 H29 O1 Br1	435.1329
LIN	C29 H27 O4 Br1	517.102
LIN	C5 H1 O3 Cl1 Br2	300.79082
LIN	C5 H3 O1 S1 Cl1 Br2	302.78871
LIN	C5 H3 O1 S1 Cl2 Br1	258.83923
NOR	C11 H10 O7 Cl2	322.97309
NOR	C11 H13 O6 S1 Br1	350.95435
NOR	C12 H11 O6 Cl1	285.01714
NOR	C12 H11 O8 Cl1	317.00697
NOR	C12 H12 O9 Cl2	368.97857
NOR	C12 H15 O7 Cl1	305.04336

NOR	C12 H9 O7 Cl1	298.99641
NOR	C13 H10 O8 Cl2	362.968
NOR	C13 H10 O9 Cl2	378.96292
NOR	C13 H11 O9 Cl1	345.00189
NOR	C13 H15 O5 Cl1	285.05353
NOR	C13 H15 O8 Cl1	333.03827
NOR	C13 H9 O7 Cl1	310.99641
NOR	C14 H11 O8 Cl1	341.00697
NOR	C14 H12 O10 Cl2	408.97348
NOR	C14 H14 O7 Cl2	363.00439
NOR	C14 H15 O5 Cl1	297.05353
NOR	C14 H9 O7 Cl1	322.99641
NOR	C15 H12 O7 Cl2	372.98874
NOR	C15 H14 O10 Cl2	422.98913
NOR	C15 H14 O7 Cl2	375.00439
NOR	C15 H15 O6 Cl1	325.04844
NOR	C15 H17 O10 Cl1	391.04375
NOR	C15 H28 O3 Cl1 Br1	369.08376
NOR	C16 H13 O7 Cl1	351.02771
NOR	C16 H14 O10 Cl2	434.98913
NOR	C16 H16 O9 Cl2	421.00987
NOR	C16 H17 O7 Br1	399.00849
NOR	C16 H19 O10 Cl1	405.0594
NOR	C16 H19 O7 Br1	401.02414
NOR	C16 H23 O6 Cl1	345.11104
NOR	C17 H13 O11 Cl1	427.00737
NOR	C17 H14 O11 Cl2	462.98405
NOR	C17 H14 O9 Cl2	430.99422
NOR	C17 H16 O8 Cl2	417.01495
NOR	C17 H17 O11 Cl1	431.03867
NOR	C17 H18 O10 Cl2	451.02043
NOR	C17 H18 O8 Cl2	419.0306
NOR	C17 H21 O8 Br1	431.03471
NOR	C17 H23 O6 Cl1	357.11104
NOR	C17 H34 O2 Cl1 Br1	383.1358
NOR	C18 H17 O11 Cl1	443.03867
NOR	C18 H19 O7 Cl1	381.07466
NOR	C18 H23 O8 Br1	445.05036
NOR	C18 H23 O8 Cl1	401.10087
NOR	C18 H25 O7 Cl1	387.12161
NOR	C18 H25 O8 Cl1	403.11652
NOR	C19 H13 O10 Cl1	435.01245
NOR	C19 H17 O10 Cl1	439.04375
NOR	C20 H19 O11 Cl1	469.05432
NOR	C20 H29 O7 Cl1	415.15291
NOR	C22 H33 O1 Cl1 Br2	505.05139
NOR	C26 H36 O1 N1 Cl2 Br1	526.12846
NOR	C5 H3 O1 S1 Cl1 Br2	302.78871

STO	C12 H10 O8 Cl2	350.968
STO	C12 H11 O6 Br1	328.96663
STO	C12 H12 O8 Cl2	352.98365
STO	C12 H12 O9 Cl2	368.97857
STO	C13 H11 O6 Cl1	297.01714
STO	C13 H11 O7 Br1	356.96154
STO	C13 H12 O9 Cl2	380.97857
STO	C13 H13 O6 Cl1	299.03279
STO	C13 H13 O7 Br1	358.97719
STO	C13 H13 O7 Cl1	315.02771
STO	C13 H14 O7 Cl2	351.00439
STO	C13 H15 O6 Cl1	301.04844
STO	C13 H15 O8 Cl1	333.03827
STO	C13 H16 O7 Cl2	353.02004
STO	C13 H9 O8 Cl1	326.99132
STO	C14 H10 O8 Cl2	374.968
STO	C14 H11 O9 Cl1	357.00189
STO	C14 H12 O8 Cl2	376.98365
STO	C14 H12 O9 Cl2	392.97857
STO	C14 H13 O7 Br1	370.97719
STO	C14 H13 O9 Cl1	359.01754
STO	C14 H14 O10 Cl2	410.98913
STO	C14 H14 O8 Cl2	378.9993
STO	C14 H14 O9 Cl2	394.99422
STO	C14 H15 O10 Cl1	377.0281
STO	C14 H15 O5 Cl1	297.05353
STO	C14 H15 O6 Br1	356.99793
STO	C14 H15 O7 Br1	372.99284
STO	C14 H17 O8 Cl1	347.05392
STO	C15 H11 O9 Cl1	369.00189
STO	C15 H12 O10 Cl2	420.97348
STO	C15 H12 O9 Cl2	404.97857
STO	C15 H13 O8 Br1	398.97211
STO	C15 H13 O9 Cl1	371.01754
STO	C15 H14 O8 Cl2	390.9993
STO	C15 H14 O9 Cl2	406.99422
STO	C15 H15 O6 Br1	368.99793
STO	C15 H15 O6 Cl1	325.04844
STO	C15 H15 O7 Br1	384.99284
STO	C15 H15 O8 Br1	400.98776
STO	C15 H16 O8 Cl2	393.01495
STO	C15 H17 O6 Br1	371.01358
STO	C15 H30 O3 Cl1 Br1	371.09941
STO	C16 H11 O9 Cl1	381.00189
STO	C16 H13 O8 Cl1	367.02262
STO	C16 H14 O10 Cl2	434.98913
STO	C16 H17 O10 Cl1	403.04375
STO	C16 H17 O6 Cl1	339.06409

STO	C16 H17 O7 Br1	399.00849
STO	C16 H17 O8 Br1	415.00341
STO	C16 H19 O8 Br1	417.01906
STO	C17 H15 O9 Cl1	397.03319
STO	C17 H19 O9 Br1	445.01397
STO	C17 H21 O7 Br1	415.03979
STO	C17 H21 O9 Cl1	403.08014
STO	C17 H34 O1 S1 Cl1 Br1	399.11295
STO	C18 H17 O11 Cl1	443.03867
STO	C18 H17 O8 Cl1	395.05392
STO	C18 H19 O9 Br1	457.01397
STO	C18 H21 O10 Cl1	431.07505
STO	C18 H21 O6 Cl1	367.09539
STO	C18 H21 O7 Br1	427.03979
STO	C18 H23 O7 Br1	429.05544
STO	C18 H23 O8 Br1	445.05036
STO	C18 H25 O8 Cl1	403.11652
STO	C19 H21 O8 Cl1	411.08522
STO	C19 H23 O10 Cl1	445.0907
STO	C19 H23 O9 Cl1	429.09579
STO	C19 H25 O8 Cl1	415.11652
STO	C20 H19 O11 Cl1	469.05432
STO	C20 H23 O9 Cl1	441.09579
STO	C25 H32 O1 N1 Cl2 Br1	510.09716
STO	C28 H40 O1 N1 Cl2 Br1	554.15976
STO	C29 H40 O1 N1 Cl2 Br1	566.15976
STO	C29 H42 O1 N1 Cl2 Br1	568.17541
STO	C30 H46 O1 N1 Cl2 Br1	584.20671
STO	C30 H47 O9 S1 Cl3	687.19336
STO	C5 H1 O3 Cl1 Br2	300.79082
STO	C5 H3 O1 S1 Br3	346.7382
MAL	C13 H11 O7 Br1	356.96154
MAL	C13 H11 O7 Br1	356.96154
MAL	C13 H13 O7 Br1	358.97719
MAL	C13 H13 O8 Br1	374.97211
MAL	C13 H15 O6 Br1	344.99793
MAL	C14 H11 O7 Br1	368.96154
MAL	C14 H11 O8 Br1	384.95646
MAL	C14 H13 O6 Br1	354.98228
MAL	C14 H13 O7 Br1	370.97719
MAL	C14 H13 O8 Br1	386.97211
MAL	C14 H13 O9 Br1	402.96702
MAL	C14 H15 O6 Br1	356.99793
MAL	C14 H15 O7 Br1	372.99284
MAL	C14 H15 O8 Br1	388.98776
MAL	C14 H17 O6 Br1	359.01358
MAL	C14 H17 O7 Br1	375.00849
MAL	C15 H11 O8 Br1	396.95646

MAL	C15 H13 O10 Br1	430.96194
MAL	C15 H13 O6 Br1	366.98228
MAL	C15 H13 O7 Br1	382.97719
MAL	C15 H13 O8 Br1	398.97211
MAL	C15 H13 O9 Br1	414.96702
MAL	C15 H15 O5 Br1	353.00301
MAL	C15 H15 O6 Br1	368.99793
MAL	C15 H15 O7 Br1	384.99284
MAL	C15 H15 O8 Br1	400.98776
MAL	C15 H15 O9 Br1	416.98267
MAL	C15 H17 O5 Br1	355.01866
MAL	C15 H17 O6 Br1	371.01358
MAL	C15 H17 O7 Br1	387.00849
MAL	C15 H17 O8 Br1	403.00341
MAL	C15 H17 O8 S1 Br1	434.97548
MAL	C15 H19 O6 Br1	373.02923
MAL	C15 H31 O10 N1 S1 Cl2	486.0973
MAL	C16 H11 O9 Br1	424.95137
MAL	C16 H13 O7 Br1	394.97719
MAL	C16 H13 O8 Br1	410.97211
MAL	C16 H13 O9 Br1	426.96702
MAL	C16 H15 O10 Br1	444.97759
MAL	C16 H15 O6 Br1	380.99793
MAL	C16 H15 O7 Br1	396.99284
MAL	C16 H15 O8 Br1	412.98776
MAL	C16 H15 O9 Br1	428.98267
MAL	C16 H15 O9 Cl1	385.03319
MAL	C16 H17 O6 Br1	383.01358
MAL	C16 H17 O7 Br1	399.00849
MAL	C16 H17 O8 Br1	415.00341
MAL	C16 H17 O9 Br1	430.99832
MAL	C16 H17 O9 Cl1	387.04884
MAL	C16 H19 O6 Br1	385.02923
MAL	C16 H19 O7 Br1	401.02414
MAL	C16 H19 O8 Br1	417.01906
MAL	C16 H19 O9 Br1	433.01397
MAL	C16 H21 O6 Br1	387.04488
MAL	C16 H21 O7 Br1	403.03979
MAL	C17 H13 O10 Br1	454.96194
MAL	C17 H13 O7 Br1	406.97719
MAL	C17 H13 O8 Br1	422.97211
MAL	C17 H13 O9 Br1	438.96702
MAL	C17 H15 O10 Br1	456.97759
MAL	C17 H15 O7 Br1	408.99284
MAL	C17 H15 O8 Br1	424.98776
MAL	C17 H15 O9 Br1	440.98267
MAL	C17 H15 O9 Cl1	397.03319
MAL	C17 H17 O10 Br1	458.99324

MAL	C17 H17 O6 Br1	395.01358
MAL	C17 H17 O7 Br1	411.00849
MAL	C17 H17 O8 Br1	427.00341
MAL	C17 H17 O9 Br1	442.99832
MAL	C17 H19 O10 Br1	461.00889
MAL	C17 H19 O7 Br1	413.02414
MAL	C17 H19 O8 Br1	429.01906
MAL	C17 H19 O9 Br1	445.01397
MAL	C17 H21 O6 Br1	399.04488
MAL	C17 H21 O7 Br1	415.03979
MAL	C17 H21 O8 Br1	431.03471
MAL	C17 H21 O9 Br1	447.02962
MAL	C18 H13 O8 Br1	434.97211
MAL	C18 H13 O9 Br1	450.96702
MAL	C18 H15 O10 Br1	468.97759
MAL	C18 H15 O7 Br1	420.99284
MAL	C18 H15 O8 Br1	436.98776
MAL	C18 H15 O9 Br1	452.98267
MAL	C18 H17 O10 Br1	470.99324
MAL	C18 H17 O11 Br1	486.98815
MAL	C18 H17 O8 Br1	439.00341
MAL	C18 H17 O9 Br1	454.99832
MAL	C18 H19 O10 Br1	473.00889
MAL	C18 H19 O7 Br1	425.02414
MAL	C18 H19 O8 Br1	441.01906
MAL	C18 H19 O9 Br1	457.01397
MAL	C18 H21 O6 Br1	411.04488
MAL	C18 H21 O7 Br1	427.03979
MAL	C18 H21 O8 Br1	443.03471
MAL	C18 H21 O9 Br1	459.02962
MAL	C18 H23 O7 Br1	429.05544
MAL	C18 H23 O8 Br1	445.05036
MAL	C18 H23 O9 Br1	461.04527
MAL	C19 H15 O10 Br1	480.97759
MAL	C19 H15 O9 Br1	464.98267
MAL	C19 H17 O10 Br1	482.99324
MAL	C19 H17 O7 Br1	435.00849
MAL	C19 H17 O8 Br1	451.00341
MAL	C19 H17 O9 Br1	466.99832
MAL	C19 H19 O10 Br1	485.00889
MAL	C19 H19 O8 Br1	453.01906
MAL	C19 H21 O10 Br1	487.02454
MAL	C19 H21 O7 Br1	439.03979
MAL	C19 H21 O8 Br1	455.03471
MAL	C19 H21 O9 Br1	471.02962
MAL	C19 H23 O6 Br1	425.06053
MAL	C19 H23 O7 Br1	441.05544
MAL	C19 H23 O8 Br1	457.05036



MAL	C19 H23 O9 Br1	473.04527
MAL	C19 H25 O7 Br1	443.07109
MAL	C20 H19 O9 Br1	481.01397
MAL	C20 H21 O10 Br1	499.02454
MAL	C20 H21 O8 Br1	467.03471
MAL	C20 H21 O9 Br1	483.02962
MAL	C20 H23 O9 Br1	485.04527
MAL	C21 H21 O11 Br1	527.01945
MAL	C21 H23 O9 Br1	497.04527
MAL	C23 H32 O1 N1 Cl2 Br1	486.09716
MAL	C25 H36 O1 N1 Cl2 Br1	514.12846
MAL	C26 H32 O1 N1 Cl2 Br1	522.09716
MAL	C27 H23 O5 Cl1	461.11613
MAL	C30 H40 O3 N1 Cl2 Br1	610.14959
MAL	C5 H1 O3 Br3	344.74031
MAL	C5 H1 O3 Cl1 Br2	300.79082
MAL	C5 H3 O1 S1 Br3	346.7382
MAL	C5 H3 O1 S1 Cl1 Br2	302.78871
MAL	C7 H7 O5 Br1	248.94041