Formation of chlorinated disinfection by-products and fate of their precursors in individual processes of a conventional water treatment plant assessed by a high-resolution mass spectrometry

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Contents in this Supporting Information.

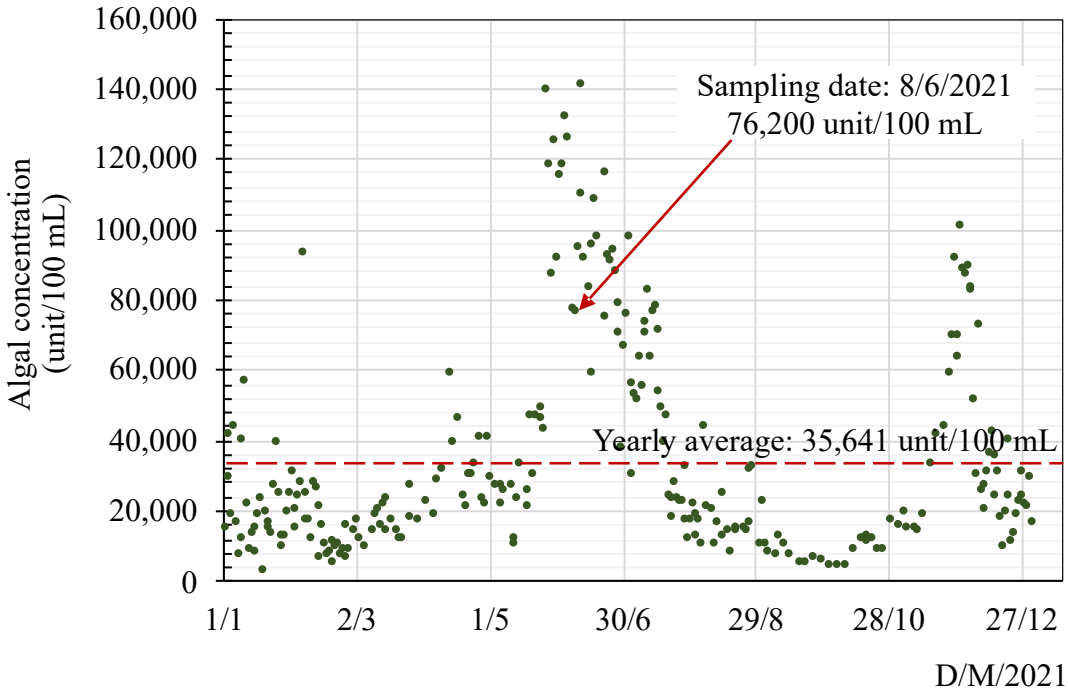

Figure S1 Algal concentrations in raw water of Bangkhen Water Treatment Plant in 2021

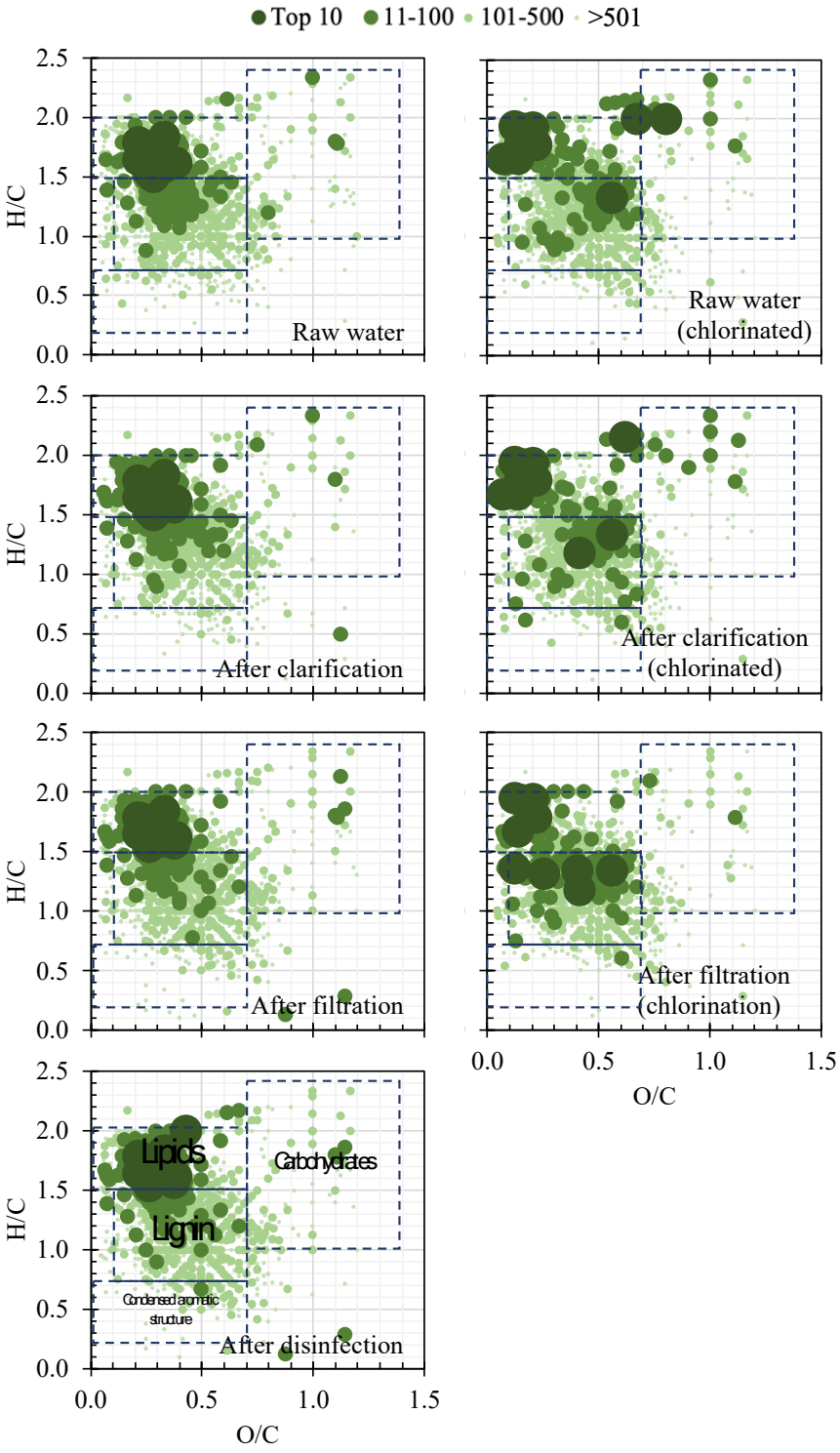

Figure S2 van Krevelen diagram of CHO components in BK-WTP (left) before chlorination, and (right) after chlorination

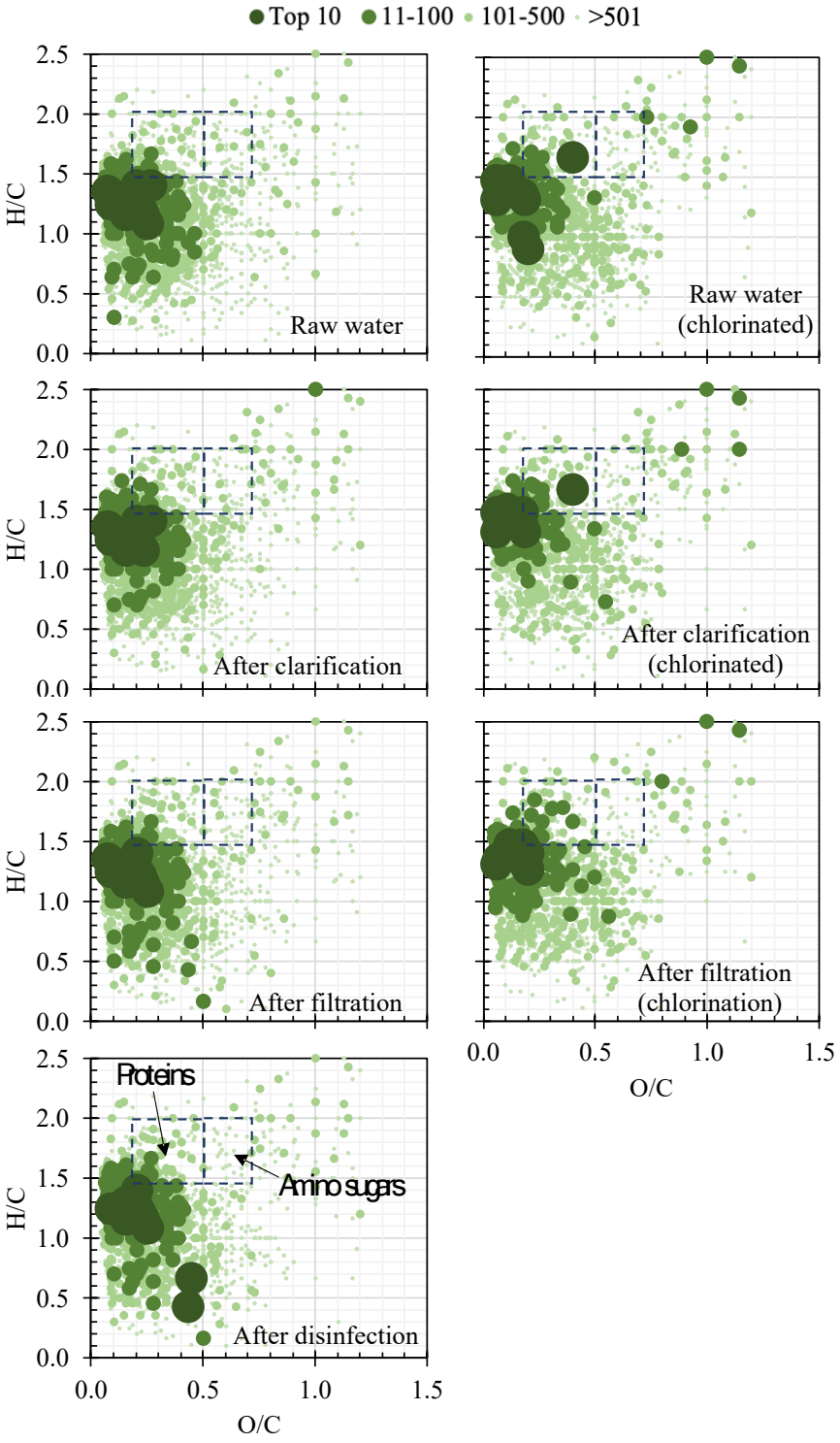

Figure S3 van Krevelen diagram of CHON components in BK-WTP (left) before chlorination, and (right) after chlorination

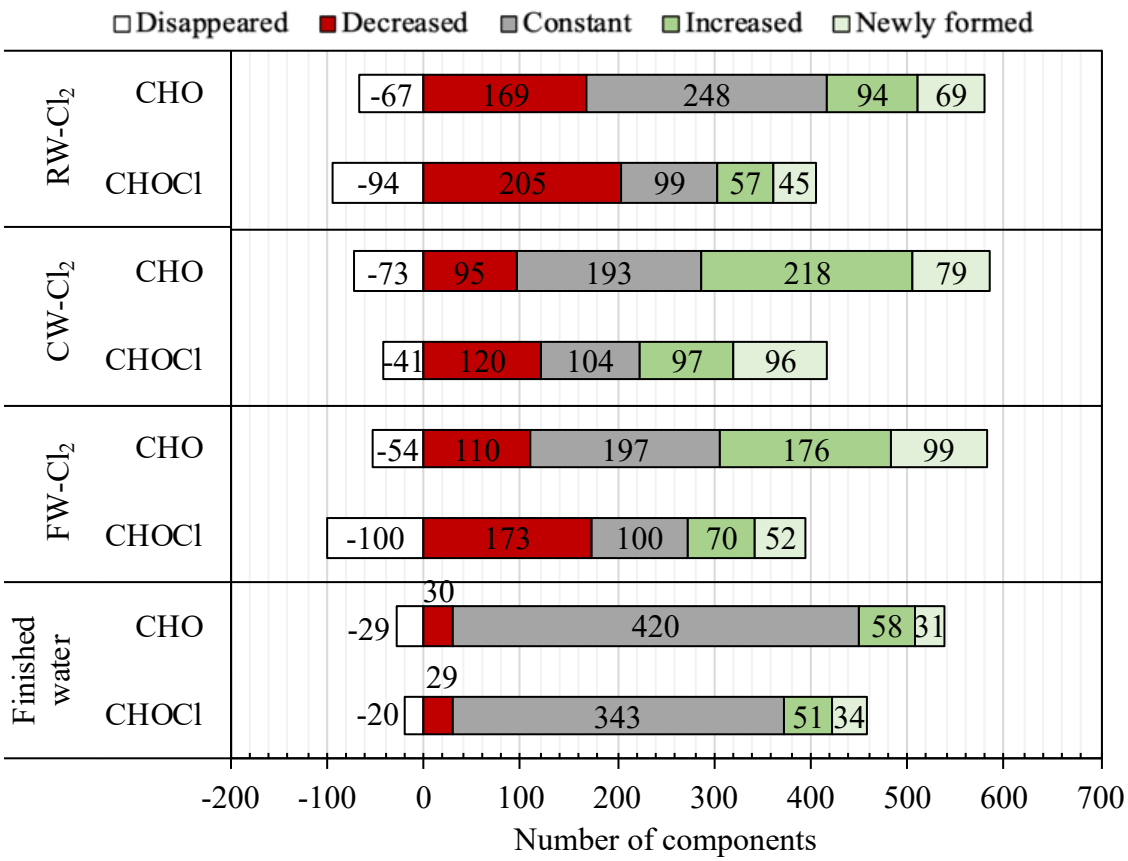

Figure S4 Changes of CHO and CHOCl components during water treatment processes

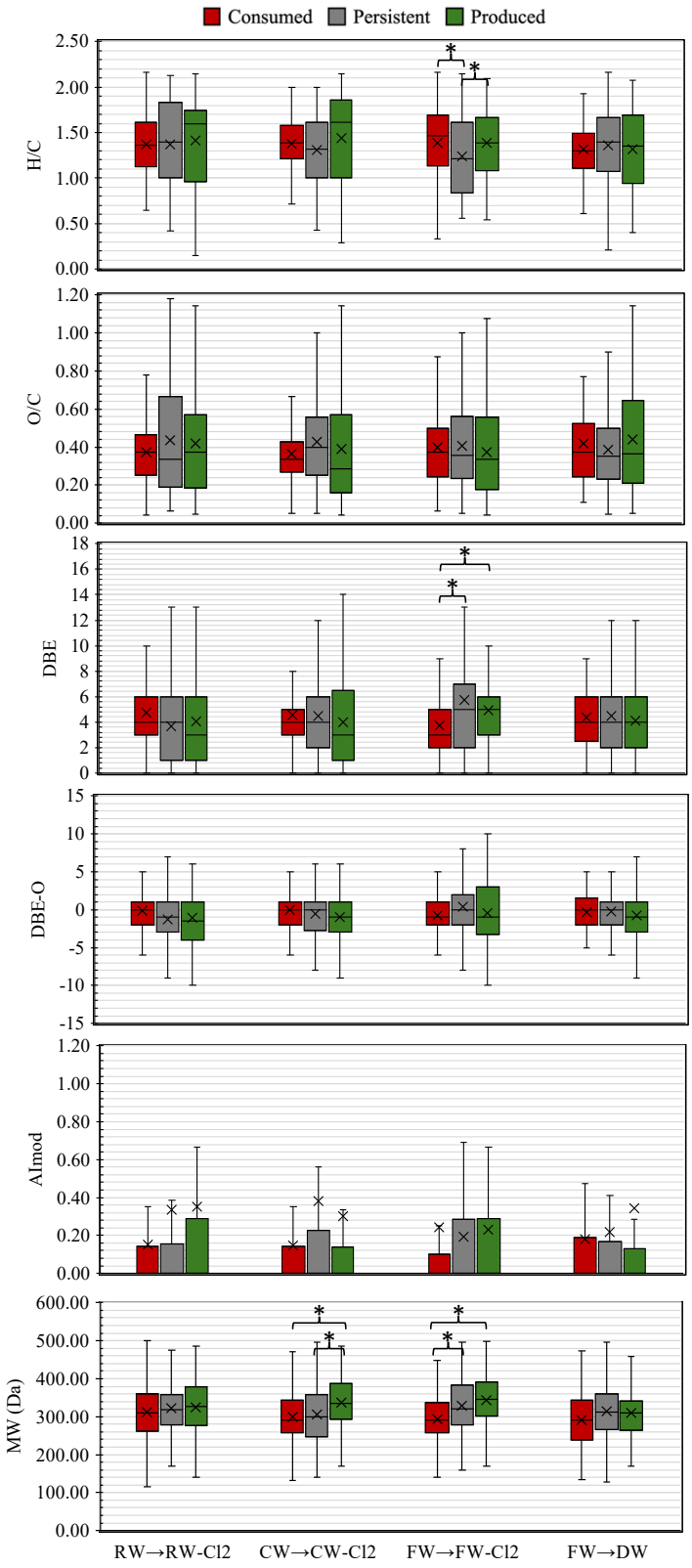

Figure S5 Molecular characteristics of CHOCl components classified into consumed, persistent, and produced after chlorination

(Asterix * indicates significant difference (p-value<0.05)

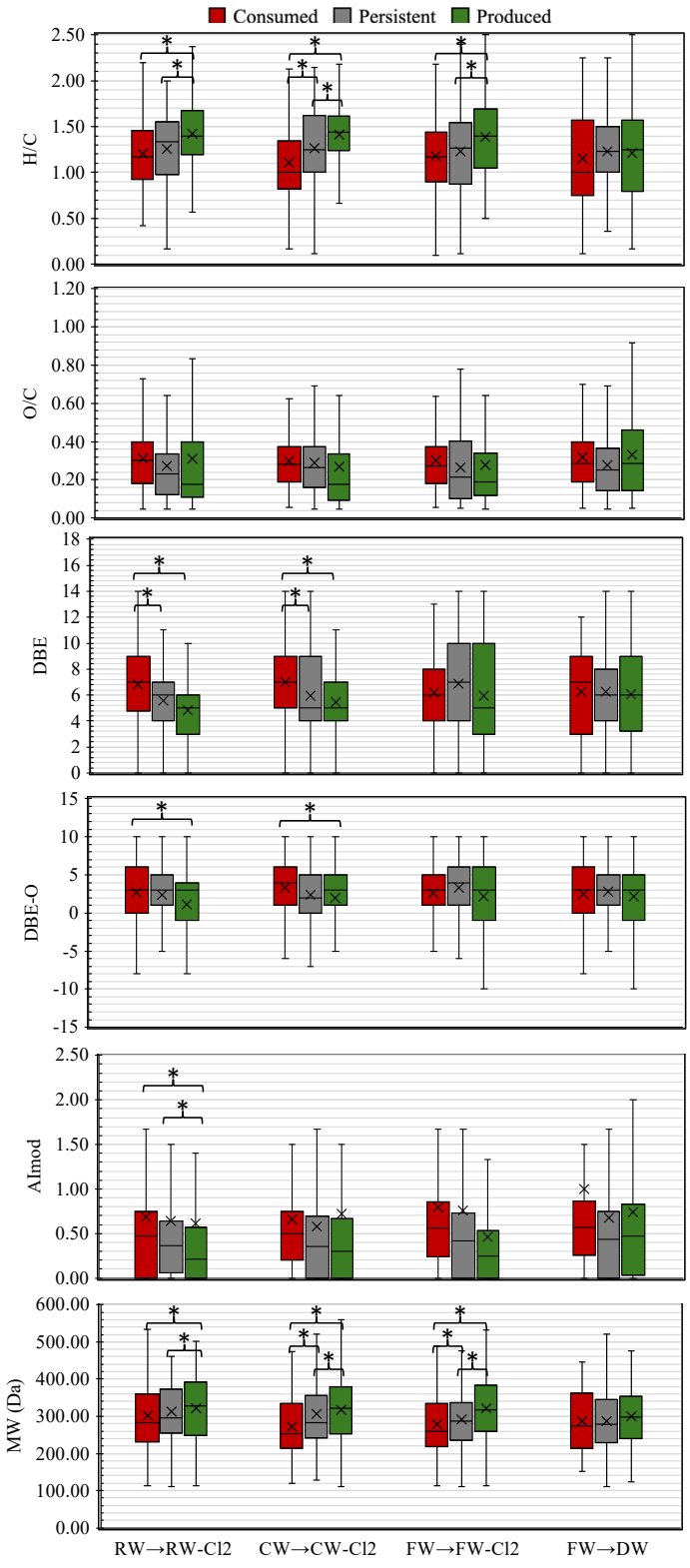

Figure S6 Molecular characteristics of CHONCl components classified into consumed, persistent, and produced after chlorination

(Asterix * indicates significant difference (p-value<0.05)

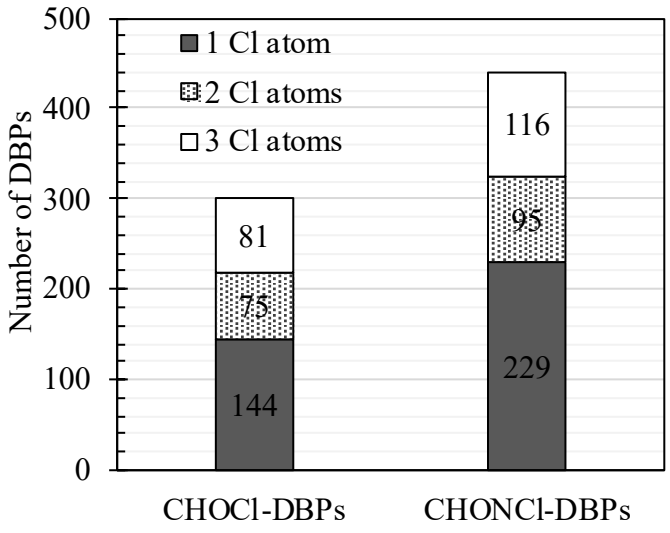

Figure S7 Number of chlorine atoms in DBPs observed in this study

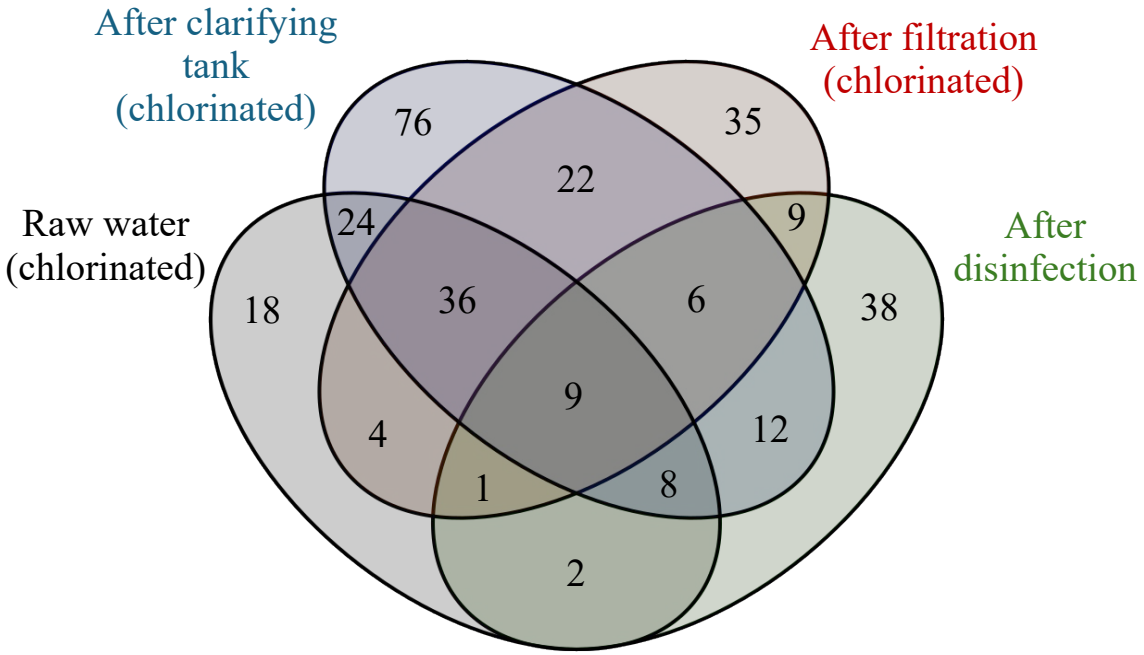

Figure S8 Venn diagram of CHOCl-DBP components detected in chlorinated samples and finished water

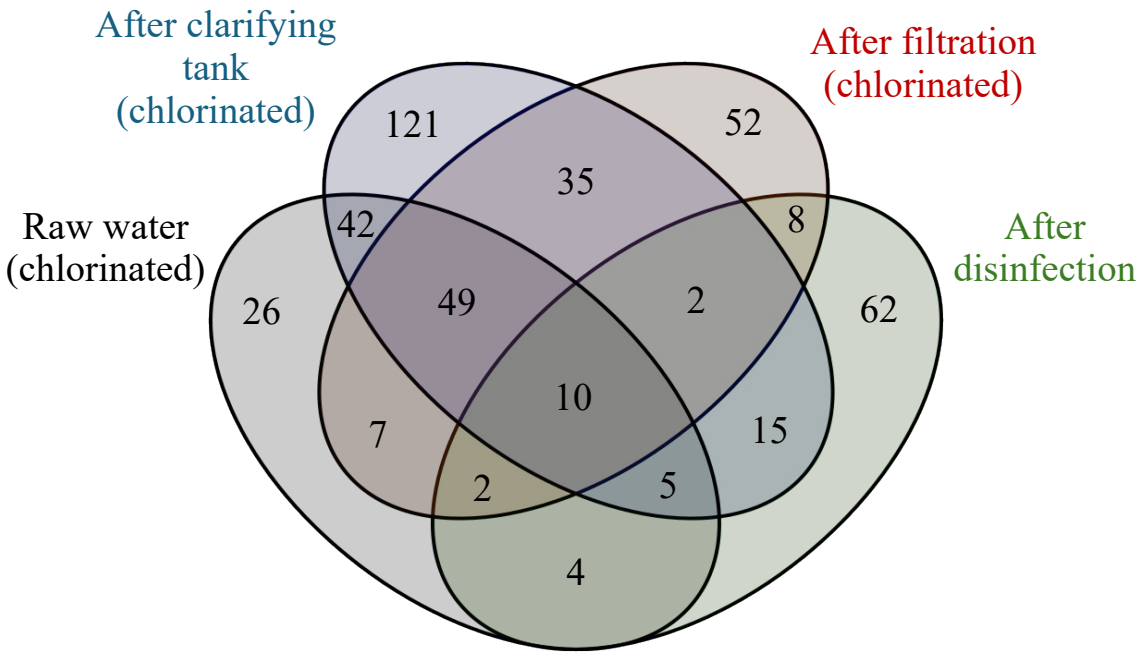

Figure S9 Venn diagram of CHONCl-DBP components detected in chlorinated samples and finished water

Table S1 Molecular characteristics of CHO, CHOCl, CHON, and CHONCl components in raw water sample

Molecular characteristics	CHO and CHOCl	CHON and CHONCl	Welch's t-test at 5% significant level
Number	1033	1340	-
H/C	1.28	1.16	<0.05
O/C	0.44	0.37	0.21
DBE	5.67	7.32	<0.05
DBE-O	-0.12	2.55	<0.05
AI_{mod}	0.29	0.52	<0.05
MW	303.10	313.01	0.08

Table S2 Number of components, total absolute intensity, and number-average molecular characteristics of CHO/CHOCl and CHON/CHONCl during water treatment processes

	RW		CW		FW		Finished water	
	CHO and CHOCl	CHON and CHONCl	CHO and CHOCl	CHON and CHONCl	CHO and CHOCl	CHON and CHONCl	CHO and CHOCl	CHON and CHONCl
Number of components	1033	1340	941	1012	980	1223	996	1249
Total Abs. intensity ($\times 10^{10}$)	1.19	2.47	0.49	0.87	0.61	1.22	0.60	1.18
H/C	1.28	1.16	1.28	1.16	1.27	1.13	1.28	1.13
O/C	0.44	0.37	0.44	0.35	0.44	0.36	0.44	0.37
DBE	5.67	7.32	5.68	7.14	5.60	7.19	5.53	7.19
DBE-O	-0.12	2.55	-0.12	2.77	-0.07	2.76	-0.15	2.65
AI_{mod}	0.29	0.52	0.23	0.53	0.23	0.55	0.24	0.54
MW	303.10	313.01	297.79	302.02	297.57	301.65	298.60	302.43

Table S3 Dissolved organic carbon (DOC) concentrations and specific UV absorbance (SUVA) of the samples before and after chlorination

Samples	DOC conc. (mg L^{-1})		SUVA (L mg^{-1} m^{-1})	
	Before Cl_2	After Cl_2	Before Cl_2	After Cl_2
RW	6.3	5.2	1.47	0.91
CW	3.5	3.4	1.99	0.74
FW	3.5	3.6	1.36	0.56
Finished water	3.8	-	1.52	-

Table S4 CHO-DBPs detected in chlorinated samples and finished water in this study. RW-Cl_2, CW-Cl_2, and FW-Cl_2 denote chlorinated raw water, chlorinated clarified water, and chlorinated filtered water, respectively.

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study				Also reported in reference(s)
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water	
$C_{13}H_{15}OCl$	222.0811	✓	✓	✓	✓	
$C_{12}H_{17}O_6Cl$	292.0714	✓	✓	✓	✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_9H_{16}O_7Cl_2$	306.0273	✓	✓	✓	✓	
$C_{18}H_{11}O_3Cl$	310.0397	✓	✓	✓	✓	
$C_{17}H_{23}O_3Cl$	310.1336	✓	✓	✓	✓	
$C_{15}H_{23}O_5Cl$	318.1234	✓	✓	✓	✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_{11}H_{19}O_9Cl$	330.0718	✓	✓	✓	✓	
$C_{14}H_{23}O_7Cl$	338.1132	✓	✓	✓	✓	Lavonen et al. (2013)
$C_{21}H_{40}O_2Cl_2$	394.2405	✓	✓	✓	✓	
$C_8H_7O_2Cl$	170.0135		✓	✓	✓	
$C_6H_8O_2Cl_2$	181.9901	✓	✓		✓	
$C_7H_{12}OCl_2$	182.0265	✓	✓	✓		
$C_{13}H_{21}OCl$	228.1281	✓	✓	✓		
$C_7H_{14}O_4Cl_2$	232.0269	✓	✓	✓		
$C_{12}H_9O_3Cl$	236.0240	✓	✓	✓		
$C_{12}H_{11}O_4Cl$	254.0346	✓	✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_6H_3O_5Cl_3$	259.9046	✓	✓		✓	
$C_{10}H_{19}OCl_3$	260.0501	✓	✓		✓	
$C_{11}H_{21}O_5Cl$	268.1078	✓	✓	✓		
$C_{11}H_{21}OCl_3$	274.0658	✓	✓		✓	
$C_{14}H_{13}O_4Cl$	280.0502		✓	✓	✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_{11}H_{19}O_6Cl$	282.0870	✓	✓	✓		
$C_{10}H_8O_6Cl_2$	293.9698	✓	✓		✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_{12}H_{11}O_7Cl$	302.0193		✓	✓	✓	Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{12}H_{17}O_7Cl$	308.0663	✓	✓	✓		Lavonen et al. (2013)
$C_{14}H_{11}O_6Cl$	310.0244	✓	✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{13}H_{21}O_2Cl_3$	314.0607	✓	✓		✓	
$C_{17}H_{19}O_4Cl$	322.0972	✓	✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{16}H_{31}O_4Cl$	322.1911	✓	✓	✓		
$C_8H_5O_8Cl_3$	333.9050	✓	✓		✓	
$C_{14}H_{21}O_7Cl$	336.0976	✓		✓	✓	Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{15}H_{25}O_2Cl_3$	342.0920	✓	✓	✓		
$C_{18}H_{15}O_5Cl$	346.0608	✓	✓	✓		
$C_{15}H_{23}O_7Cl$	350.1132	✓	✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{16}H_{27}O_6Cl$	350.1496	✓	✓	✓		Lavonen et al. (2013)

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study				Also reported in reference(s)
		$RW\text{-}Cl_2$	$CW\text{-}Cl_2$	$FW\text{-}Cl_2$	Finished water	
$C_{14}H_{23}O_8Cl$	354.1081	✓	✓	✓		
$C_{17}H_{25}O_6Cl$	360.1340	✓	✓	✓		Lavonen et al. (2013), Zhang et al. (2014), Phungsai et al. (2018)
$C_{18}H_{31}O_5Cl$	362.1860	✓	✓	✓		
$C_{17}H_{13}O_7Cl$	364.0350	✓	✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{18}H_{17}O_6Cl$	364.0714	✓	✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{15}H_{23}O_8Cl$	366.1081	✓	✓	✓		Lavonen et al. (2013)
$C_{17}H_{33}O_2Cl_3$	374.1546	✓	✓	✓		
$C_{16}H_{23}O_8Cl$	378.1081	✓	✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{14}H_{26}O_8Cl_2$	392.1005	✓	✓	✓		
$C_{16}H_{31}O_4Cl_3$	392.1288	✓	✓	✓		
$C_{14}H_{29}O_{10}Cl$	392.1449		✓	✓	✓	
$C_{18}H_{29}O_7Cl$	392.1602	✓	✓	✓		Lavonen et al. (2013)
$C_{17}H_{27}O_8Cl$	394.1394	✓	✓	✓		Lavonen et al. (2013)
$C_{18}H_{29}O_3Cl_3$	398.1182	✓	✓	✓		
$C_{22}H_{21}OCl_3$	406.0658	✓	✓	✓		
$C_{14}H_{27}O_{11}Cl$	406.1242		✓	✓	✓	
$C_{17}H_{33}O_4Cl_3$	406.1444		✓	✓	✓	
$C_{13}H_{22}O_{10}Cl_2$	408.0590	✓	✓	✓		
$C_{24}H_{24}O_2Cl_2$	414.1153	✓	✓	✓		
$C_{18}H_{33}O_4Cl_3$	418.1444	✓	✓		✓	
$C_{14}H_{25}O_{12}Cl$	420.1035	✓	✓	✓		
$C_{13}H_{17}O_{14}Cl$	432.0307	✓	✓	✓		
$C_{16}H_{30}O_9Cl_2$	436.1267	✓	✓	✓		
$C_{26}H_{25}O_4Cl$	436.1441	✓	✓	✓		
$C_{22}H_{37}O_5Cl_3$	486.1707	✓	✓	✓		
$C_5H_8O_2Cl_2$	169.9901	✓			✓	
$C_9H_5O_4Cl$	211.9876		✓		✓	
$C_{13}H_7OCl$	214.0185		✓	✓		
$C_9H_{12}O_2Cl_2$	222.0214	✓	✓			
$C_{12}H_{12}OCl_2$	242.0265			✓	✓	
$C_7H_{15}O_7Cl$	246.0506	✓	✓			
$C_7H_5O_8Cl$	251.9673			✓	✓	
$C_{16}H_{15}OCl$	258.0811		✓		✓	
$C_9H_5O_7Cl$	259.9724	✓	✓			Zhang et al. (2014)
$C_{14}H_{13}O_3Cl$	264.0553		✓	✓		
$C_{16}H_{27}OCl$	270.1750		✓		✓	
$C_{11}H_{19}OCl_3$	272.0501	✓	✓			
$C_{11}H_8O_4Cl_2$	273.9800			✓	✓	Lavonen et al. (2013), Zhang et al. (2014)

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study				Also reported in reference(s)
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water	
$C_{14}H_{27}O_3Cl$	278.1649	✓	✓			
$C_{13}H_9O_5Cl$	280.0139	✓	✓			Lavonen et al. (2013), Zhang et al. (2014)
$C_7H_2O_8Cl_2$	283.9127	✓	✓			
$C_{12}H_9O_6Cl$	284.0088	✓	✓			Lavonen et al. (2013), Andersson et al. (2021)
$C_8H_5O_5Cl_3$	285.9203	✓	✓			
$C_{11}H_{11}O_7Cl$	290.0193		✓	✓		Lavonen et al. (2013), Zhang et al. (2014), Phungsai et al. (2018)
$C_{17}H_{23}O_2Cl$	294.1387			✓	✓	
$C_{13}H_{11}O_6Cl$	298.0244	✓	✓			Lavonen et al. (2013), Andersson et al. (2021)
$C_{13}H_{21}OCl_3$	298.0658	✓	✓			
$C_{12}H_{13}O_7Cl$	304.0350		✓	✓		Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{10}H_8O_7Cl_2$	309.9647		✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{10}H_{19}O_9Cl$	318.0718	✓	✓			
$C_{11}H_{23}O_8Cl$	318.1081		✓	✓		
$C_{12}H_{15}O_8Cl$	322.0455		✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{12}H_{17}O_8Cl$	324.0612	✓	✓			Lavonen et al. (2013)
$C_{15}H_{25}OCl_3$	326.0971	✓	✓			
$C_{16}H_{21}O_5Cl$	328.1078			✓	✓	Lavonen et al. (2013)
$C_{15}H_{27}OCl_3$	328.1127	✓	✓			
$C_9H_8O_9Cl_2$	329.9545	✓	✓			
$C_{12}H_9O_9Cl$	331.9935		✓		✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_{14}H_{27}O_2Cl_3$	332.1077		✓		✓	
$C_{12}H_{25}O_8Cl$	332.1238		✓	✓		
$C_{10}H_{19}O_{10}Cl$	334.0667		✓		✓	
$C_{15}H_{20}O_4Cl_2$	334.0739			✓	✓	
$C_{17}H_{34}O_2Cl_2$	340.1936	✓	✓			
$C_{14}H_{23}O_3Cl_3$	344.0713		✓		✓	
$C_{12}H_{25}O_9Cl$	348.1187	✓	✓			
$C_{13}H_{14}O_7Cl_2$	352.0117		✓	✓		Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{11}H_{22}O_8Cl_2$	352.0692		✓	✓		
$C_{16}H_{31}O_2Cl_3$	360.1390	✓	✓			
$C_{15}H_{19}O_8Cl$	362.0768		✓	✓		Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{15}H_{29}O_3Cl_3$	362.1182		✓	✓		
$C_{14}H_{19}O_9Cl$	366.0718		✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{17}H_{17}O_7Cl$	368.0663		✓	✓		Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{16}H_{29}O_7Cl$	368.1602	✓	✓			
$C_{14}H_{17}O_5Cl_3$	370.0142			✓	✓	
$C_{16}H_{29}O_3Cl_3$	374.1182	✓	✓			

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study				Also reported in reference(s)
		$RW\text{-}Cl_2$	$CW\text{-}Cl_2$	$FW\text{-}Cl_2$	Finished water	
$C_{15}H_{27}O_4Cl_3$	376.0975		✓		✓	
$C_{16}H_{31}O_3Cl_3$	376.1339		✓		✓	
$C_{17}H_{27}O_7Cl$	378.1445	✓		✓		Lavonen et al. (2013)
$C_{19}H_{25}O_6Cl$	384.1340	✓		✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{17}H_{33}O_3Cl_3$	390.1495		✓		✓	
$C_{17}H_{20}O_7Cl_2$	406.0586		✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{15}H_{31}O_{10}Cl$	406.1606		✓	✓		
$C_{18}H_{29}O_8Cl$	408.1551	✓	✓			Lavonen et al. (2013)
$C_{12}H_{20}O_{11}Cl_2$	410.0383	✓			✓	
$C_{19}H_{35}O_3Cl_3$	416.1652		✓	✓		
$C_{23}H_{23}OCl_3$	420.0814		✓	✓		
$C_{18}H_{35}O_4Cl_3$	420.1601		✓		✓	
$C_{16}H_{16}O_9Cl_2$	422.0171		✓	✓		Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{19}H_{33}O_4Cl_3$	430.1444	✓	✓			
$C_{13}H_{19}O_{14}Cl$	434.0463		✓		✓	
$C_{18}H_{23}O_{10}Cl$	434.0980		✓	✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{26}H_{26}O_3Cl_2$	456.1259	✓	✓			
$C_{24}H_{24}O_5Cl_2$	462.1001			✓	✓	
$C_{26}H_{26}O_4Cl_2$	472.1208		✓	✓		
$C_{21}H_{35}O_5Cl_3$	472.1550	✓		✓		
$C_{22}H_{35}O_5Cl_3$	484.1550		✓	✓		
$C_{21}H_{33}O_6Cl_3$	486.1343	✓		✓		
$C_{21}H_{29}O_7Cl_3$	498.0979			✓	✓	
$C_2H_2O_2Cl_2$	127.9432		✓			
$C_4H_6OCl_2$	139.9796	✓				
$C_5H_8OCl_2$	153.9952	✓				
$C_8H_9O_2Cl$	172.0291			✓		
$C_7H_7O_3Cl$	174.0084				✓	
$C_5H_6O_3Cl_2$	183.9694				✓	
$C_6H_{10}O_2Cl_2$	184.0058	✓				
$C_7H_3O_4Cl$	185.9720				✓	
$C_{11}H_9OCl$	192.0342	✓				
$C_{11}H_{13}OCl$	196.0655	✓				
$C_{11}H_9O_2Cl$	208.0291	✓				
$C_9H_7O_4Cl$	214.0033	✓				Gonsior et al. (2014)
$C_7H_3O_2Cl_3$	223.9199		✓			
$C_8H_9OCl_3$	225.9719				✓	
$C_{14}H_9OCl$	228.0342		✓			

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study				Also reported in reference(s)
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water	
$C_8H_5O_6Cl$	231.9775				✓	
$C_{10}H_{15}O_4Cl$	234.0659				✓	
$C_8H_8O_4Cl_2$	237.9800				✓	
$C_{14}H_{19}OCl$	238.1124			✓		
$C_7H_{10}O_5Cl_2$	243.9905				✓	
$C_9H_9O_6Cl$	248.0088				✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_{10}H_{13}O_5Cl$	248.0452	✓				Zhang et al. (2014)
$C_{11}H_{17}O_4Cl$	248.0815				✓	
$C_8H_6O_5Cl_2$	251.9592				✓	
$C_{15}H_{21}OCl$	252.1281			✓		
$C_{13}H_{16}OCl_2$	258.0578			✓		
$C_{10}H_6O_4Cl_2$	259.9643		✓			Zhang et al. (2014)
$C_{10}H_9O_6Cl$	260.0088		✓			Lavonen et al. (2013), Zhang et al. (2014)
$C_7H_{13}O_8Cl$	260.0299	✓				
$C_{14}H_{25}O_2Cl$	260.1543		✓			
$C_{13}H_{22}OCl_2$	264.1048		✓			
$C_9H_8O_5Cl_2$	265.9749				✓	Zhang et al. (2014)
$C_8H_6O_6Cl_2$	267.9541				✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_8H_9O_8Cl$	267.9986				✓	
$C_{14}H_{21}O_3Cl$	272.1179				✓	
$C_{10}H_9O_7Cl$	276.0037			✓		Lavonen et al. (2013), Zhang et al. (2014), Phungsai et al. (2018)
$C_{10}H_{19}O_2Cl_3$	276.0451				✓	
$C_{15}H_{13}O_3Cl$	276.0553		✓			
$C_{12}H_{17}O_5Cl$	276.0765			✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{13}H_{21}O_4Cl$	276.1128			✓		Lavonen et al. (2013)
$C_{10}H_{11}O_7Cl$	278.0193				✓	Lavonen et al. (2013), Phungsai et al. (2018)
$C_{17}H_{23}OCl$	278.1437			✓		
$C_{14}H_{26}OCl_2$	280.1361		✓			
$C_{17}H_{11}O_2Cl$	282.0448				✓	
$C_{11}H_5O_7Cl$	283.9724	✓				
$C_{11}H_{15}O_2Cl_3$	284.0138				✓	
$C_{12}H_{22}O_3Cl_2$	284.0946		✓			
$C_{12}H_{11}O_6Cl$	286.0244		✓			Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{10}H_{15}O_3Cl_3$	288.0087				✓	
$C_8H_{13}O_9Cl$	288.0248	✓				
$C_{11}H_{19}O_2Cl_3$	288.0451		✓			
$C_{13}H_{17}O_5Cl$	288.0765				✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_7H_5O_6Cl_3$	289.9152		✓			

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study				Also reported in reference(s)
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water	
$C_{11}H_{21}O_2Cl_3$	290.0607		✓			
$C_{15}H_{27}O_3Cl$	290.1649		✓			
$C_8H_{17}O_9Cl$	292.0561		✓			
$C_{16}H_{17}O_3Cl$	292.0866		✓			
$C_{12}H_{13}O_2Cl_3$	293.9981			✓		
$C_{10}H_{11}O_8Cl$	294.0142		✓			Zhang et al. (2014)
$C_{15}H_{28}OCl_2$	294.1517		✓			
$C_{13}H_9O_6Cl$	296.0088		✓			Lavonen et al. (2013), Zhang et al. (2014)
$C_8H_4O_8Cl_2$	297.9283		✓			
$C_{10}H_{12}O_6Cl_2$	298.0011				✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_{15}H_{20}O_2Cl_2$	302.0840			✓		
$C_{18}H_{19}O_2Cl$	302.1074			✓		
$C_{16}H_{24}OCl_2$	302.1204			✓		
$C_{11}H_{22}O_5Cl_2$	304.0844				✓	
$C_{14}H_{21}O_5Cl$	304.1078		✓			Lavonen et al. (2013), Zhang et al. (2014)
$C_{11}H_8O_6Cl_2$	305.9698		✓			Lavonen et al. (2013), Zhang et al. (2014)
$C_{11}H_{11}O_8Cl$	306.0142		✓			Lavonen et al. (2013), Zhang et al. (2014)
$C_{16}H_{28}OCl_2$	306.1517		✓			
$C_{19}H_{29}OCl$	308.1907			✓		
$C_{14}H_{21}OCl_3$	310.0658		✓			
$C_{12}H_2O_6Cl_2$	311.9228			✓		
$C_{13}H_{22}O_4Cl_2$	312.0895				✓	
$C_{16}H_{21}O_4Cl$	312.1128			✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{17}H_{25}O_3Cl$	312.1492			✓		
$C_{12}H_{23}O_7Cl$	314.1132		✓			
$C_{13}H_{13}O_7Cl$	316.0350		✓			Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{18}H_{14}OCl_2$	316.0422		✓			
$C_{13}H_{23}O_2Cl_3$	316.0764		✓			
$C_{14}H_{27}OCl_3$	316.1127		✓			
$C_{12}H_{25}O_7Cl$	316.1289			✓		
$C_9H_{15}O_{10}Cl$	318.0354				✓	
$C_{13}H_{15}O_7Cl$	318.0506		✓			Lavonen et al. (2013), Zhang et al. (2014), Phungsai et al. (2018), Andersson et al. (2021)
$C_{13}H_{25}O_2Cl_3$	318.0920		✓			
$C_8H_7O_7Cl_3$	319.9257	✓				
$C_{11}H_{19}O_4Cl_3$	320.0349				✓	
$C_{12}H_{23}O_3Cl_3$	320.0713				✓	
$C_{10}H_4O_8Cl_2$	321.9283				✓	

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study				Also reported in reference(s)
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water	
$C_{11}H_8O_7Cl_2$	321.9647	✓				Lavonen et al. (2013), Zhang et al. (2014)
$C_{18}H_{25}O_3Cl$	324.1492			✓		
$C_{16}H_{30}O_2Cl_2$	324.1623		✓			
$C_{10}H_8O_8Cl_2$	325.9596				✓	
$C_{14}H_{21}O_2Cl_3$	326.0607		✓			
$C_{18}H_{27}O_3Cl$	326.1649			✓		
$C_{16}H_{32}O_2Cl_2$	326.1779		✓			
$C_{12}H_5O_9Cl$	327.9622		✓			Lavonen et al. (2013), Zhang et al. (2014)
$C_{14}H_{25}O_2Cl_3$	330.0920		✓			
$C_{13}H_{23}O_3Cl_3$	332.0713		✓			
$C_{19}H_{18}OCl_2$	332.0735				✓	
$C_{12}H_{10}O_7Cl_2$	335.9804		✓			Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{12}H_{13}O_9Cl$	336.0248			✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{17}H_{30}O_2Cl_2$	336.1623		✓			
$C_{11}H_{10}O_8Cl_2$	339.9753				✓	Lavonen et al. (2013), Zhang et al. (2014)
$C_{12}H_{14}O_7Cl_2$	340.0117				✓	Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{11}H_{13}O_{10}Cl$	340.0197			✓		
$C_{10}H_{19}O_6Cl_3$	340.0247		✓			
$C_{18}H_{25}O_4Cl$	340.1441			✓		Lavonen et al. (2013)
$C_{16}H_{30}O_3Cl_2$	340.1572		✓			
$C_{16}H_{19}O_6Cl$	342.0870				✓	Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{16}H_{32}O_3Cl_2$	342.1729		✓			
$C_{17}H_{25}O_5Cl$	344.1391			✓		Lavonen et al. (2013)
$C_{14}H_{15}O_8Cl$	346.0455		✓			Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{15}H_{19}O_7Cl$	346.0819		✓			Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{14}H_{25}O_3Cl_3$	346.0869		✓			
$C_{15}H_{29}O_2Cl_3$	346.1233		✓			
$C_{19}H_{34}OCl_2$	348.1987		✓			
$C_{12}H_{10}O_8Cl_2$	351.9753		✓			Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{12}H_{23}O_5Cl_3$	352.0611				✓	
$C_{15}H_{25}O_7Cl$	352.1289	✓				Lavonen et al. (2013)
$C_{14}H_{17}O_4Cl_3$	354.0192			✓		
$C_{13}H_2O_8Cl_2$	355.9127	✓				
$C_9H_{18}O_{10}Cl_2$	356.0277		✓			
$C_{15}H_{13}O_8Cl$	356.0299		✓			Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{18}H_{25}O_5Cl$	356.1391			✓		Lavonen et al. (2013)
$C_{15}H_{25}O_3Cl_3$	358.0869		✓			

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study				Also reported in reference(s)
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water	
$C_{14}H_{27}O_8Cl$	358.1394			✓		
$C_{19}H_{30}O_2Cl_2$	360.1623			✓		
$C_{14}H_{25}O_4Cl_3$	362.0818		✓			
$C_{14}H_{14}O_7Cl_2$	364.0117		✓			Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{16}H_{19}O_3Cl_3$	364.0400			✓		
$C_{16}H_{21}O_3Cl_3$	366.0556			✓		
$C_{16}H_{27}O_7Cl$	366.1445			✓		Lavonen et al. (2013)
$C_{17}H_{30}O_4Cl_2$	368.1521		✓			
$C_{20}H_{29}O_4Cl$	368.1754				✓	Lavonen et al. (2013)
$C_{16}H_{17}O_8Cl$	372.0612		✓			Lavonen et al. (2013), Zhang et al. (2014), Andersson et al. (2021)
$C_{18}H_{27}O_6Cl$	374.1496			✓		Lavonen et al. (2013), Andersson et al. (2021)
$C_{11}H_{22}O_{10}Cl_2$	384.0590		✓			
$C_{17}H_{29}O_3Cl_3$	386.1182		✓			
$C_{19}H_{37}OCl_3$	386.1910		✓			
$C_{16}H_{27}O_4Cl_3$	388.0975		✓			
$C_{17}H_{31}O_3Cl_3$	388.1339		✓			
$C_{18}H_{35}O_2Cl_3$	388.1703		✓			
$C_{19}H_{36}O_4Cl_2$	398.1991	✓				
$C_{20}H_{29}O_6Cl$	400.1653		✓			Lavonen et al. (2013)
$C_{17}H_{29}O_4Cl_3$	402.1131		✓			
$C_{19}H_{37}O_2Cl_3$	402.1859		✓			
$C_{18}H_{36}O_5Cl_2$	402.1940			✓		
$C_{17}H_{31}O_4Cl_3$	404.1288		✓			
$C_{18}H_{35}O_3Cl_3$	404.1652		✓			
$C_{17}H_{25}O_5Cl_3$	414.0768				✓	
$C_{19}H_{33}O_3Cl_3$	414.1495		✓			
$C_{19}H_{37}O_3Cl_3$	418.1808		✓			
$C_{17}H_{23}O_{10}Cl$	422.0980			✓		Lavonen et al. (2013), Zhang et al. (2014)
$C_{17}H_{19}O_6Cl_3$	424.0247			✓		
$C_{25}H_{27}O_4Cl$	426.1598		✓			
$C_{18}H_{33}O_5Cl_3$	434.1394		✓			
$C_{17}H_{33}O_6Cl_3$	438.1343	✓				
$C_{19}H_{31}O_9Cl$	438.1657			✓		
$C_{18}H_{33}O_6Cl_3$	450.1343		✓			
$C_{19}H_{29}O_6Cl_3$	458.1030				✓	
$C_{24}H_{23}O_7Cl$	458.1132				✓	
$C_{25}H_{17}O_7Cl$	464.0663		✓			
$C_{24}H_{17}O_8Cl$	468.0612		✓			

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study				Also reported in reference(s)
		$RW\text{-}Cl_2$	$CW\text{-}Cl_2$	$FW\text{-}Cl_2$	Finished water	
$C_{19}H_{25}O_7Cl_3$	470.0666	✓				
$C_{15}H_{21}O_{15}Cl$	476.0569		✓			

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Table S5 CHON-DBPs detected in chlorinated samples and finished water in this study. RW-Cl_2, CW-Cl_2, and FW-Cl_2 denote chlorinated raw water, chlorinated clarified water, and chlorinated filtered water, respectively.

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{12}H_{15}ON_2Cl_3$	308.0250	✓	✓	✓	✓
$C_{14}H_{17}O_2N_2Cl_3$	350.0356	✓	✓	✓	✓
$C_{12}H_{26}O_6N_2Cl_2$	364.1168	✓	✓	✓	✓
$C_{15}H_{21}O_2N_2Cl_3$	366.0669	✓	✓	✓	✓
$C_{12}H_{25}O_4N_2Cl_3$	366.0880	✓	✓	✓	✓
$C_{16}H_{23}O_3N_2Cl_3$	396.0774	✓	✓	✓	✓
$C_{11}H_{20}O_{10}N_2Cl_2$	410.0495	✓	✓	✓	✓
$C_{18}H_{25}O_3N_2Cl_3$	422.0931	✓	✓	✓	✓
$C_{14}H_{27}O_{12}N_2Cl$	450.1253	✓	✓	✓	✓
$C_{15}H_{31}O_{11}N_2Cl$	450.1616	✓	✓	✓	✓
$C_6H_6ON_2Cl_2$	191.9857	✓	✓	✓	
$C_7H_{12}O_2NCl_3$	246.9934	✓	✓	✓	
$C_{11}H_{12}ON_2Cl_2$	258.0327	✓	✓		✓
$C_9H_{14}O_3N_2Cl_2$	268.0381		✓	✓	✓
$C_9H_{19}ON_2Cl_3$	276.0563	✓	✓	✓	
$C_9H_{17}O_2N_2Cl_3$	290.0356	✓	✓	✓	
$C_{14}H_7O_4N_2Cl$	302.0094		✓	✓	✓
$C_{11}H_{15}O_2N_2Cl_3$	312.0199	✓	✓	✓	
$C_{15}H_{18}ON_2Cl_2$	312.0796	✓	✓	✓	
$C_{13}H_{17}ON_2Cl_3$	322.0406	✓	✓	✓	
$C_{12}H_{19}O_2N_2Cl_3$	328.0512	✓	✓	✓	
$C_{12}H_{21}O_2N_2Cl_3$	330.0669	✓	✓	✓	
$C_{13}H_{17}O_2N_2Cl_3$	338.0356	✓	✓	✓	
$C_{20}H_{21}ON_2Cl$	340.1342	✓		✓	✓
$C_{17}H_{26}ON_2Cl_2$	344.1422	✓	✓		✓
$C_{15}H_{19}ON_2Cl_3$	348.0563	✓	✓	✓	
$C_{15}H_{21}ON_2Cl_3$	350.0719	✓	✓	✓	
$C_{14}H_{19}O_2N_2Cl_3$	352.0512	✓	✓	✓	
$C_{15}H_{25}ON_2Cl_3$	354.1032	✓	✓	✓	
$C_{17}H_{24}O_2N_2Cl_2$	358.1215	✓	✓	✓	
$C_{21}H_{31}ON_2Cl$	362.2125	✓	✓	✓	
$C_{15}H_{19}O_2N_2Cl_3$	364.0512	✓		✓	✓
$C_{15}H_{25}O_6N_2Cl$	364.1401	✓	✓	✓	
$C_{13}H_{15}O_4N_2Cl_3$	368.0097	✓	✓		✓
$C_{14}H_{19}O_3N_2Cl_3$	368.0461	✓	✓	✓	
$C_{15}H_{23}O_2N_2Cl_3$	368.0825	✓	✓	✓	

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{10}H_{21}O_9NCl_2$	369.0593	✓	✓	✓	
$C_{18}H_{26}O_2N_2Cl_2$	372.1371	✓	✓		✓
$C_{19}H_{30}ON_2Cl_2$	372.1735	✓	✓	✓	
$C_{17}H_{25}ON_2Cl_3$	378.1032	✓	✓	✓	
$C_{11}H_{22}O_{11}NCl$	379.0881	✓	✓	✓	
$C_{15}H_{19}O_3N_2Cl_3$	380.0461	✓	✓	✓	
$C_{16}H_{23}O_2N_2Cl_3$	380.0825	✓	✓	✓	
$C_{16}H_{25}O_2N_2Cl_3$	382.0982	✓	✓	✓	
$C_{19}H_{28}O_2N_2Cl_2$	386.1528	✓	✓		✓
$C_{17}H_{21}O_2N_2Cl_3$	390.0669	✓	✓	✓	
$C_{18}H_{25}ON_2Cl_3$	390.1032	✓	✓	✓	
$C_{16}H_{21}O_3N_2Cl_3$	394.0618	✓	✓	✓	
$C_{17}H_{25}O_2N_2Cl_3$	394.0982	✓	✓	✓	
$C_{11}H_{23}O_{11}N_2Cl$	394.0990	✓	✓	✓	
$C_{11}H_{22}O_9N_2Cl_2$	396.0702	✓	✓	✓	
$C_{19}H_{32}O_3N_2Cl_2$	406.1790	✓	✓	✓	
$C_{17}H_{25}O_3N_2Cl_3$	410.0931	✓	✓	✓	
$C_{16}H_{23}O_4N_2Cl_3$	412.0723	✓	✓	✓	
$C_{22}H_{22}O_2N_2Cl_2$	416.1058	✓	✓	✓	
$C_{19}H_{25}O_2N_2Cl_3$	418.0982	✓	✓	✓	
$C_{13}H_{25}O_{11}N_2Cl$	420.1147	✓	✓	✓	
$C_{17}H_{23}O_4N_2Cl_3$	424.0723	✓	✓	✓	
$C_{18}H_{27}O_3N_2Cl_3$	424.1087	✓	✓	✓	
$C_{18}H_{19}O_8N_2Cl$	426.0830	✓	✓	✓	
$C_{22}H_{20}O_3N_2Cl_2$	430.0851	✓	✓	✓	
$C_{13}H_{23}O_{12}N_2Cl$	434.0940	✓	✓	✓	
$C_{13}H_{25}O_{12}N_2Cl$	436.1096	✓	✓	✓	
$C_{20}H_{29}O_3N_2Cl_3$	450.1244	✓	✓	✓	
$C_{15}H_{29}O_{12}N_2Cl$	464.1409	✓	✓	✓	
$C_{19}H_{29}O_5N_2Cl_3$	470.1142	✓	✓	✓	
$C_{21}H_{26}O_{10}NCl$	487.1245	✓	✓	✓	
$C_{14}H_{17}O_{11}N_2Cl_3$	493.9898	✓	✓	✓	
$C_5H_7O_2N_2Cl$	162.0196	✓	✓		
$C_6H_1O_2N_2Cl$	167.9727		✓		✓
$C_2H_5O_2N_2Cl_3$	193.9417			✓	✓
$C_6H_6O_2N_2Cl_2$	207.9806	✓	✓		
$C_7H_3O_4N_2Cl$	213.9781	✓	✓		
$C_8H_8O_4NCl$	217.0142		✓		✓
$C_9H_1O_4N_2Cl$	235.9625	✓	✓		

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_9H_{11}O_4N_2Cl$	246.0407			✓	✓
$C_8H_5O_4NCl_2$	248.9596	✓			✓
$C_8H_{10}O_3N_2Cl_2$	252.0068		✓	✓	
$C_{11}H_{14}ON_2Cl_2$	260.0483		✓		✓
$C_{11}H_{18}ON_2Cl_2$	264.0796		✓		✓
$C_9H_{12}O_3N_2Cl_2$	266.0225	✓	✓		
$C_{14}H_7O_2N_2Cl$	270.0196		✓	✓	
$C_{15}H_{21}ON_2Cl$	280.1342		✓	✓	
$C_{10}H_{13}ON_2Cl_3$	282.0093	✓			✓
$C_{13}H_{17}O_3N_2Cl$	284.0928		✓		✓
$C_{17}H_{16}ONCl$	285.0920	✓		✓	
$C_9H_{15}O_2N_2Cl_3$	288.0199		✓	✓	
$C_{13}H_{18}ON_2Cl_2$	288.0796	✓	✓		
$C_8H_{19}O_7N_2Cl$	290.0881	✓	✓		
$C_8H_{15}O_3N_2Cl_3$	292.0148		✓	✓	
$C_{14}H_{10}ON_2Cl_2$	292.0170		✓	✓	
$C_7H_{17}O_8N_2Cl$	292.0673		✓	✓	
$C_{12}H_{18}O_2N_2Cl_2$	292.0745	✓	✓		
$C_6H_{14}O_7N_2Cl_2$	296.0178	✓	✓		
$C_{10}H_{13}O_2N_2Cl_3$	298.0043	✓	✓		
$C_{17}H_{15}ON_2Cl$	298.0873	✓		✓	
$C_{18}H_{18}ONCl$	299.1077	✓		✓	
$C_{16}H_{13}O_2N_2Cl$	300.0666			✓	✓
$C_{14}H_{18}ON_2Cl_2$	300.0796	✓	✓		
$C_{12}H_{22}ONCl_3$	301.0767		✓		✓
$C_{14}H_{22}ON_2Cl_2$	304.1109	✓		✓	
$C_8H_{16}O_6N_2Cl_2$	306.0385	✓	✓		
$C_8H_{18}O_6N_2Cl_2$	308.0542	✓	✓		
$C_{12}H_{19}ON_2Cl_3$	312.0563		✓	✓	
$C_{17}H_{13}O_2N_2Cl$	312.0666		✓	✓	
$C_{15}H_{23}O_3N_2Cl$	314.1397		✓		✓
$C_9H_{14}O_9NCl$	315.0357	✓	✓		
$C_{15}H_{22}ON_2Cl_2$	316.1109		✓		✓
$C_{15}H_{24}ON_2Cl_2$	318.1266	✓	✓		
$C_{12}H_{13}O_2N_2Cl_3$	322.0043	✓	✓		
$C_{12}H_{15}O_2N_2Cl_3$	324.0199	✓			✓
$C_{13}H_{19}ON_2Cl_3$	324.0563	✓	✓		
$C_{11}H_{13}O_3N_2Cl_3$	325.9992	✓	✓		
$C_{13}H_{21}ON_2Cl_3$	326.0719		✓	✓	

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{17}H_{27}O_2N_2Cl$	326.1761	✓	✓		
$C_{12}H_{24}O_7NCl$	329.1241	✓	✓		
$C_{16}H_{27}O_3N_2Cl$	330.1710	✓	✓		
$C_{10}H_{17}O_4N_2Cl_3$	334.0254			✓	✓
$C_{16}H_{12}O_2N_2Cl_2$	334.0276			✓	✓
$C_{14}H_{17}ON_2Cl_3$	334.0406		✓	✓	
$C_{15}H_{24}O_2N_2Cl_2$	334.1215	✓	✓		
$C_{19}H_{27}ON_2Cl$	334.1812		✓	✓	
$C_9H_{21}O_9N_2Cl$	336.0936	✓	✓		
$C_{15}H_{26}O_2N_2Cl_2$	336.1371	✓	✓		
$C_{18}H_{25}O_2N_2Cl$	336.1605	✓	✓		
$C_{19}H_{29}ON_2Cl$	336.1968		✓	✓	
$C_{12}H_{13}O_3N_2Cl_3$	337.9992	✓	✓		
$C_{12}H_{15}O_3N_2Cl_3$	340.0148	✓	✓		
$C_{18}H_{13}O_3N_2Cl$	340.0615		✓		✓
$C_{17}H_{22}ON_2Cl_2$	340.1109	✓	✓		
$C_{16}H_9O_5N_2Cl$	344.0200		✓	✓	
$C_{16}H_{21}O_3NCl_2$	345.0899			✓	✓
$C_{16}H_{11}O_5N_2Cl$	346.0357		✓	✓	
$C_{13}H_{24}O_3NCl_3$	347.0822		✓		✓
$C_{19}H_{25}O_2N_2Cl$	348.1605		✓		✓
$C_{20}H_{31}ON_2Cl$	350.2125		✓	✓	
$C_{14}H_{21}O_2N_2Cl_3$	354.0669		✓	✓	
$C_{18}H_{26}ON_2Cl_2$	356.1422	✓	✓		
$C_{12}H_7O_9N_2Cl$	357.9840		✓	✓	
$C_{19}H_{19}O_3N_2Cl$	358.1084			✓	✓
$C_{16}H_{19}ON_2Cl_3$	360.0563		✓	✓	
$C_{16}H_{21}ON_2Cl_3$	362.0719		✓	✓	
$C_{10}H_{19}O_{10}N_2Cl$	362.0728	✓	✓		
$C_{14}H_{15}O_3N_2Cl_3$	364.0148	✓	✓		
$C_{15}H_{22}O_4N_2Cl_2$	364.0957		✓	✓	
$C_{19}H_{25}O_3N_2Cl$	364.1554	✓	✓		
$C_{16}H_{29}O_5N_2Cl$	364.1765	✓		✓	
$C_{16}H_{25}ON_2Cl_3$	366.1032		✓	✓	
$C_{19}H_{29}O_3N_2Cl$	368.1867		✓		✓
$C_{22}H_{31}ON_2Cl$	374.2125		✓	✓	
$C_{16}H_{19}O_2N_2Cl_3$	376.0512	✓	✓		
$C_{17}H_{23}ON_2Cl_3$	376.0876	✓	✓		
$C_{14}H_{25}O_8N_2Cl$	384.1299		✓		✓

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{12}H_{23}O_{10}N_2Cl$	390.1041	✓	✓		
$C_{11}H_{21}O_{11}N_2Cl$	392.0834	✓	✓		
$C_{15}H_{24}O_9NCl$	397.1140		✓		✓
$C_{18}H_{17}O_2N_2Cl_3$	398.0356		✓	✓	
$C_{22}H_{23}O_3N_2Cl$	398.1397		✓	✓	
$C_{10}H_{19}O_8N_2Cl_3$	400.0207	✓			✓
$C_{20}H_{30}O_2N_2Cl_2$	400.1684	✓	✓		
$C_{17}H_9O_8N_2Cl$	404.0047		✓	✓	
$C_{18}H_{13}O_7N_2Cl$	404.0411		✓	✓	
$C_{18}H_{25}O_2N_2Cl_3$	406.0982		✓	✓	
$C_{19}H_{29}ON_2Cl_3$	406.1345	✓	✓		
$C_{14}H_{31}O_9N_2Cl$	406.1718	✓		✓	
$C_{17}H_{23}O_3N_2Cl_3$	408.0774	✓	✓		
$C_{20}H_{25}O_5N_2Cl$	408.1452		✓	✓	
$C_{16}H_{21}O_4N_2Cl_3$	410.0567	✓		✓	
$C_{19}H_{25}O_6N_2Cl$	412.1401		✓		✓
$C_{21}H_{18}O_3N_2Cl_2$	416.0694	✓	✓		
$C_{19}H_{23}O_2N_2Cl_3$	416.0825		✓	✓	
$C_{19}H_{29}O_2N_2Cl_3$	422.1295	✓	✓		
$C_{16}H_{27}O_9N_2Cl$	426.1405		✓	✓	
$C_{14}H_{26}O_9N_2Cl_2$	436.1015		✓	✓	
$C_{18}H_{27}O_4N_2Cl_3$	440.1036		✓	✓	
$C_{18}H_{16}O_7N_2Cl_2$	442.0335		✓	✓	
$C_{15}H_{27}O_{11}N_2Cl$	446.1303	✓	✓		
$C_{13}H_{22}O_{11}N_2Cl_2$	452.0601		✓	✓	
$C_{19}H_{33}O_{11}N_2Cl$	500.1773			✓	✓
$C_5H_6O_2NCl$	147.0087		✓		
$C_5H_1ONCl_2$	160.9435				✓
$C_6H_8O_2NCl$	161.0244				✓
$C_7H_9ON_2Cl$	172.0403				✓
$C_8H_5ON_2Cl$	180.0090			✓	
$C_6H_1O_3N_2Cl$	183.9676	✓			
$C_5H_{10}ON_2Cl_2$	184.0170			✓	
$C_4H_9O_4N_2Cl$	184.0251				✓
$C_7H_4O_3NCl$	184.9880		✓		
$C_5H_1O_4N_2Cl$	187.9625				✓
$C_6H_7O_3N_2Cl$	190.0145			✓	
$C_7H_3O_3N_2Cl$	197.9832	✓			
$C_9H_{11}ON_2Cl$	198.0560		✓		

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_8H_{13}O_2N_2Cl$	204.0666		✓		
$C_8H_4O_4NCl$	212.9829		✓		
$C_{11}H_5ON_2Cl$	216.0090				✓
$C_7H_4O_2N_2Cl_2$	217.9650	✓			
$C_9H_{14}O_3NCl$	219.0662	✓			
$C_7H_8O_2N_2Cl_2$	221.9963				✓
$C_{11}H_{13}ON_2Cl$	224.0716		✓		
$C_7H_{12}O_2N_2Cl_2$	226.0276			✓	
$C_6H_7ON_2Cl_3$	227.9624	✓			
$C_9H_6ON_2Cl_2$	227.9857	✓			
$C_{11}H_{19}ON_2Cl$	230.1186		✓		
$C_{12}H_9ON_2Cl$	232.0403				✓
$C_{12}H_{11}ON_2Cl$	234.0560				✓
$C_9H_{15}O_3N_2Cl$	234.0771		✓		
$C_9H_{14}ON_2Cl_2$	236.0483				✓
$C_7H_7ON_2Cl_3$	239.9624				✓
$C_9H_4O_5NCl$	240.9778				✓
$C_{10}H_{10}ON_2Cl_2$	244.0170				✓
$C_{13}H_9ON_2Cl$	244.0403				✓
$C_{10}H_{12}ON_2Cl_2$	246.0327	✓			
$C_7H_5O_6N_2Cl$	247.9836				✓
$C_{10}H_{17}O_3N_2Cl$	248.0928		✓		
$C_8H_5ON_2Cl_3$	249.9467	✓			
$C_{13}H_{17}ON_2Cl$	252.1029		✓		
$C_{11}H_{24}O_3NCl$	253.1445		✓		
$C_7H_5O_2N_2Cl_3$	253.9417		✓		
$C_8H_{11}O_4NCl_2$	255.0065				✓
$C_{13}H_{21}ON_2Cl$	256.1342		✓		
$C_9H_7O_5N_2Cl$	258.0044				✓
$C_{12}H_{19}O_2N_2Cl$	258.1135		✓		
$C_{10}H_{10}O_2N_2Cl_2$	260.0119	✓			
$C_9H_9ON_2Cl_3$	265.9780	✓			
$C_5H_{12}O_6N_2Cl_2$	266.0072	✓			
$C_{11}H_6O_2N_2Cl_2$	267.9806				✓
$C_{12}H_{10}ON_2Cl_2$	268.0170				✓
$C_{11}H_{22}ON_2Cl_2$	268.1109		✓		
$C_{10}H_{17}O_3NCl_2$	269.0586				✓
$C_{12}H_{12}ON_2Cl_2$	270.0327	✓			
$C_{10}H_{20}O_2N_2Cl_2$	270.0902			✓	

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{14}H_{23}ON_2Cl$	270.1499		✓		
$C_{10}H_6O_6NCl$	270.9884		✓		
$C_{10}H_5O_4NCl_2$	272.9596		✓		
$C_{10}H_8O_6NCl$	273.0040		✓		
$C_{11}H_{12}O_2N_2Cl_2$	274.0276		✓		
$C_{12}H_{18}ON_2Cl_2$	276.0796		✓		
$C_{15}H_{17}ON_2Cl$	276.1029		✓		
$C_{10}H_{12}O_6NCl$	277.0353				✓
$C_9H_7O_2N_2Cl_3$	279.9573				✓
$C_{12}H_9O_4N_2Cl$	280.0251				✓
$C_{14}H_{17}O_2N_2Cl$	280.0979		✓		
$C_{12}H_{22}ON_2Cl_2$	280.1109				✓
$C_9H_6O_3NCl_3$	280.9413		✓		
$C_{11}H_{20}O_5NCl$	281.1030			✓	
$C_{12}H_{24}O_4NCl$	281.1394		✓		
$C_9H_9O_2N_2Cl_3$	281.9730	✓			
$C_{10}H_{16}O_3N_2Cl_2$	282.0538			✓	
$C_{15}H_{23}ON_2Cl$	282.1499		✓		
$C_{12}H_{10}O_5NCl$	283.0248				✓
$C_{11}H_{22}O_5NCl$	283.1187				✓
$C_{12}H_{10}O_2N_2Cl_2$	284.0119	✓			
$C_{16}H_{13}ON_2Cl$	284.0716		✓		
$C_{11}H_{22}O_2N_2Cl_2$	284.1058			✓	
$C_{15}H_{25}ON_2Cl$	284.1655		✓		
$C_{14}H_7O_3N_2Cl$	286.0145		✓		
$C_{15}H_{11}O_2N_2Cl$	286.0509			✓	
$C_{13}H_{16}ON_2Cl_2$	286.0640		✓		
$C_{16}H_{15}ON_2Cl$	286.0873			✓	
$C_{16}H_{17}ON_2Cl$	288.1029			✓	
$C_{10}H_{18}O_2NCl_3$	289.0403				✓
$C_{13}H_7O_4N_2Cl$	290.0094				✓
$C_{13}H_{20}ON_2Cl_2$	290.0953		✓		
$C_{10}H_7O_2N_2Cl_3$	291.9573				✓
$C_{12}H_5O_5N_2Cl$	291.9887		✓		
$C_{14}H_{13}O_3N_2Cl$	292.0615				✓
$C_{16}H_{21}ON_2Cl$	292.1342		✓		
$C_{12}H_7O_5N_2Cl$	294.0044				✓
$C_{16}H_{23}ON_2Cl$	294.1499		✓		
$C_{11}H_{18}O_3N_2Cl_2$	296.0694			✓	

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{16}H_{25}ON_2Cl$	296.1655		✓		
$C_{16}H_{11}O_2N_2Cl$	298.0509			✓	
$C_{13}H_{15}O_4N_2Cl$	298.0720		✓		
$C_{13}H_{17}O_4N_2Cl$	300.0877		✓		
$C_{17}H_{17}ON_2Cl$	300.1029			✓	
$C_9H_{13}O_3N_2Cl_3$	301.9992				✓
$C_{14}H_{20}ON_2Cl_2$	302.0953		✓		
$C_9H_{15}O_3N_2Cl_3$	304.0148			✓	
$C_{12}H_{17}O_5N_2Cl$	304.0826		✓		
$C_{17}H_{21}ON_2Cl$	304.1342		✓		
$C_{10}H_{18}O_3NCl_3$	305.0352				✓
$C_{12}H_{16}O_3N_2Cl_2$	306.0538		✓		
$C_{14}H_{24}ON_2Cl_2$	306.1266		✓		
$C_{17}H_{23}ON_2Cl$	306.1499		✓		
$C_{12}H_{15}O_4NCl_2$	307.0378				✓
$C_{11}H_{11}O_2N_2Cl_3$	307.9886	✓			
$C_{16}H_{21}O_2N_2Cl$	308.1292		✓		
$C_{17}H_{25}ON_2Cl$	308.1655		✓		
$C_{13}H_{24}O_2N_2Cl_2$	310.1215		✓		
$C_{16}H_{23}O_2N_2Cl$	310.1448		✓		
$C_{18}H_{17}ON_2Cl$	312.1029			✓	
$C_{11}H_{21}O_6N_2Cl$	312.1088		✓		
$C_{16}H_{25}O_2N_2Cl$	312.1605		✓		
$C_{17}H_{12}O_3NCl$	313.0506				✓
$C_{14}H_{19}O_4N_2Cl$	314.1033		✓		
$C_{12}H_7O_2N_2Cl_3$	315.9573	✓			
$C_{15}H_9O_4N_2Cl$	316.0251			✓	
$C_{16}H_{13}O_3N_2Cl$	316.0615			✓	
$C_{17}H_{17}O_2N_2Cl$	316.0979			✓	
$C_{15}H_{25}O_3N_2Cl$	316.1554		✓		
$C_{11}H_5O_3N_2Cl_3$	317.9366	✓			
$C_{13}H_{16}O_3N_2Cl_2$	318.0538		✓		
$C_{18}H_{23}ON_2Cl$	318.1499		✓		
$C_{11}H_{20}O_3NCl_3$	319.0509		✓		
$C_{12}H_{24}O_2NCl_3$	319.0873		✓		
$C_{13}H_{15}ON_2Cl_3$	320.0250		✓		
$C_{10}H_{19}O_3N_2Cl_3$	320.0461			✓	
$C_{11}H_{23}O_2N_2Cl_3$	320.0825			✓	
$C_{18}H_{25}ON_2Cl$	320.1655		✓		

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{12}H_{16}O_4N_2Cl_2$	322.0487				✓
$C_{10}H_{21}O_3N_2Cl_3$	322.0618			✓	
$C_{12}H_{19}O_6N_2Cl$	322.0932				✓
$C_{17}H_{23}O_2N_2Cl$	322.1448		✓		
$C_{18}H_{27}ON_2Cl$	322.1812		✓		
$C_{12}H_{18}O_4N_2Cl_2$	324.0644			✓	
$C_{17}H_{25}O_2N_2Cl$	324.1605		✓		
$C_{13}H_{24}O_6NCl$	325.1292				✓
$C_{12}H_{17}O_2N_2Cl_3$	326.0356	✓			
$C_{13}H_{24}O_3N_2Cl_2$	326.1164			✓	
$C_{17}H_{13}O_3N_2Cl$	328.0615			✓	
$C_{16}H_{22}ON_2Cl_2$	328.1109		✓		
$C_{16}H_{25}O_3N_2Cl$	328.1554		✓		
$C_{16}H_{11}O_4N_2Cl$	330.0407				✓
$C_{17}H_{15}O_3N_2Cl$	330.0771			✓	
$C_{10}H_{19}O_8N_2Cl$	330.0830		✓		
$C_{16}H_{24}ON_2Cl_2$	330.1266		✓		
$C_{19}H_{23}ON_2Cl$	330.1499			✓	
$C_{12}H_{20}O_3NCl_3$	331.0509		✓		
$C_{10}H_{15}O_4N_2Cl_3$	332.0097			✓	
$C_{17}H_{17}O_3N_2Cl$	332.0928			✓	
$C_{19}H_{25}ON_2Cl$	332.1655		✓		
$C_{16}H_{28}ON_2Cl_2$	334.1579		✓		
$C_{16}H_{17}O_4N_2Cl$	336.0877				✓
$C_{17}H_{21}O_3N_2Cl$	336.1241		✓		
$C_{14}H_{25}O_5N_2Cl$	336.1452			✓	
$C_{15}H_{28}O_5NCl$	337.1656		✓		
$C_{17}H_{23}O_3N_2Cl$	338.1397		✓		
$C_{18}H_{27}O_2N_2Cl$	338.1761		✓		
$C_{15}H_{11}ON_2Cl_3$	339.9937		✓		
$C_{13}H_{19}O_2N_2Cl_3$	340.0512		✓		
$C_{14}H_{23}ON_2Cl_3$	340.0876		✓		
$C_{14}H_{26}O_3N_2Cl_2$	340.1320			✓	
$C_{17}H_{25}O_3N_2Cl$	340.1554		✓		
$C_{18}H_{29}O_2N_2Cl$	340.1918		✓		
$C_{12}H_{17}O_3N_2Cl_3$	342.0305		✓		
$C_{17}H_{24}ON_2Cl_2$	342.1266		✓		
$C_{14}H_{28}O_3N_2Cl_2$	342.1477	✓			
$C_{17}H_{27}O_3N_2Cl$	342.1710		✓		

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{11}H_{15}O_4N_2Cl_3$	344.0097		✓		
$C_{18}H_{17}O_3N_2Cl$	344.0928			✓	
$C_{18}H_{33}O_2N_2Cl$	344.2231		✓		
$C_{19}H_{20}O_3NCl$	345.1132			✓	
$C_{14}H_{13}O_2N_2Cl_3$	346.0043				✓
$C_{18}H_{19}O_3N_2Cl$	346.1084		✓		
$C_{20}H_{27}ON_2Cl$	346.1812		✓		
$C_{12}H_7O_4N_2Cl_3$	347.9471				✓
$C_{18}H_{21}O_3N_2Cl$	348.1241				✓
$C_{11}H_{21}O_4N_2Cl_3$	350.0567			✓	
$C_{16}H_{15}O_5N_2Cl$	350.0670				✓
$C_{17}H_{19}O_4N_2Cl$	350.1033				✓
$C_{18}H_{23}O_3N_2Cl$	350.1397		✓		
$C_{19}H_{27}O_2N_2Cl$	350.1761		✓		
$C_{14}H_{22}O_7NCl$	351.1085				✓
$C_{17}H_{21}O_4N_2Cl$	352.1190		✓		
$C_{18}H_{25}O_3N_2Cl$	352.1554		✓		
$C_{19}H_{29}O_2N_2Cl$	352.1918		✓		
$C_{12}H_{13}O_4N_2Cl_3$	353.9941	✓			
$C_{19}H_{15}O_3N_2Cl$	354.0771				✓
$C_{14}H_{24}O_4N_2Cl_2$	354.1113			✓	
$C_{20}H_{19}O_2N_2Cl$	354.1135			✓	
$C_{18}H_{27}O_3N_2Cl$	354.1710		✓		
$C_{20}H_{21}O_2N_2Cl$	356.1292			✓	
$C_{14}H_{12}O_5N_2Cl_2$	358.0123				✓
$C_{18}H_{28}ON_2Cl_2$	358.1579		✓		
$C_{18}H_{17}O_4N_2Cl$	360.0877			✓	
$C_{10}H_3O_{11}N_2Cl$	361.9425				✓
$C_{16}H_{11}O_6N_2Cl$	362.0306				✓
$C_{14}H_{16}O_5N_2Cl_2$	362.0436			✓	
$C_{14}H_{19}O_7N_2Cl$	362.0881				✓
$C_{18}H_{19}O_4N_2Cl$	362.1033			✓	
$C_{18}H_{21}O_4N_2Cl$	364.1190		✓		
$C_{18}H_{23}O_4N_2Cl$	366.1346		✓		
$C_{19}H_{27}O_3N_2Cl$	366.1710		✓		
$C_{15}H_{20}O_3NCl_3$	367.0509		✓		
$C_{14}H_{22}O_5N_2Cl_2$	368.0906			✓	
$C_{18}H_{25}O_4N_2Cl$	368.1503				✓
$C_{16}H_{16}O_4N_2Cl_2$	370.0487			✓	

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{15}H_{15}O_7N_2Cl$	370.0568		✓		
$C_{19}H_{28}ON_2Cl_2$	370.1579		✓		
$C_{18}H_{27}O_4N_2Cl$	370.1659		✓		
$C_{19}H_{17}O_4N_2Cl$	372.0877			✓	
$C_{16}H_{21}O_6N_2Cl$	372.1088		✓		
$C_{18}H_{29}O_4N_2Cl$	372.1816	✓			
$C_{19}H_{19}O_4N_2Cl$	374.1033			✓	
$C_{12}H_{25}O_9N_2Cl$	376.1249		✓		
$C_{16}H_{11}O_7N_2Cl$	378.0255		✓		
$C_{20}H_{27}O_3N_2Cl$	378.1710	✓			
$C_{17}H_{17}O_6N_2Cl$	380.0775				✓
$C_{20}H_{29}O_3N_2Cl$	380.1867		✓		
$C_{16}H_{22}O_3NCl_3$	381.0665			✓	
$C_{11}H_{21}O_6N_2Cl_3$	382.0465			✓	
$C_{20}H_{15}O_4N_2Cl$	382.0720				✓
$C_{19}H_{29}O_4N_2Cl$	384.1816		✓		
$C_{20}H_{19}O_4N_2Cl$	386.1033			✓	
$C_{17}H_{23}O_6N_2Cl$	386.1245		✓		
$C_{21}H_{23}O_3N_2Cl$	386.1397			✓	
$C_{19}H_{31}O_4N_2Cl$	386.1972		✓		
$C_{18}H_{29}O_5N_2Cl$	388.1765	✓			
$C_{12}H_{20}O_{11}NCl$	389.0725				✓
$C_{13}H_{24}O_{10}NCl$	389.1089				✓
$C_{17}H_{11}O_7N_2Cl$	390.0255		✓		
$C_{18}H_{15}O_6N_2Cl$	390.0619				✓
$C_{20}H_{23}O_4N_2Cl$	390.1346			✓	
$C_{17}H_{27}O_6N_2Cl$	390.1558		✓		
$C_{14}H_{27}O_4N_2Cl_3$	392.1036	✓			
$C_{13}H_{25}O_8NCl_2$	393.0957				✓
$C_{17}H_9O_3N_2Cl_3$	393.9679				✓
$C_{15}H_{17}O_4N_2Cl_3$	394.0254	✓			
$C_{19}H_{27}O_5N_2Cl$	398.1609		✓		
$C_{20}H_{31}O_4N_2Cl$	398.1972		✓		
$C_{15}H_{26}O_9NCl$	399.1296		✓		
$C_{18}H_{21}O_2N_2Cl_3$	402.0669		✓		
$C_{18}H_{27}O_6N_2Cl$	402.1558				✓
$C_{12}H_{23}O_{11}N_2Cl$	406.0990		✓		
$C_{16}H_{19}O_4N_2Cl_3$	408.0410			✓	
$C_{18}H_{19}O_7N_2Cl$	410.0881				✓

DBP formula	Theo. MW (Da)	Presence(s) of DBPs in this study			
		RW-Cl_2	CW-Cl_2	FW-Cl_2	Finished water
$C_{21}H_{31}O_4N_2Cl$	410.1972		✓		
$C_{20}H_{29}O_5N_2Cl$	412.1765		✓		
$C_{20}H_{31}O_5N_2Cl$	414.1922		✓		
$C_{16}H_{30}O_9NCl$	415.1609		✓		
$C_{18}H_{21}O_3N_2Cl_3$	418.0618		✓		
$C_{14}H_{27}O_{10}N_2Cl$	418.1354		✓		
$C_{17}H_{17}O_9N_2Cl$	428.0623		✓		
$C_{17}H_{27}O_9N_2Cl$	438.1405				✓
$C_{21}H_{27}O_6N_2Cl$	438.1558		✓		
$C_{18}H_{23}O_7N_2Cl_3$	484.0571		✓		
$C_{17}H_{29}O_{13}N_2Cl$	504.1358			✓	
$C_{15}H_{19}O_{11}N_2Cl_3$	508.0054	✓			
$C_{32}H_{32}O_8NCl$	593.1816		✓		
$C_{35}H_{50}O_{12}NCl$	711.3022			✓	

Table S6 Complete list of CHO precursors and their fates during water treatment processes

Precursors	Changes in intensities between two consecutive processes			Formation mechanism	DBPs
	RW→CW	CW→FW	FW→Finished water		
$C_9H_8O_4$	Constant	Increased	Constant	ES	$C_9H_7O_4Cl$
$C_{12}H_{10}O_3$	Disappeared	Newly Formed	Constant	ES	$C_{12}H_9O_3Cl$
$C_7H_{16}O_7$	Constant	Increased	Constant	ES	$C_7H_{15}O_7Cl$
$C_{12}H_{12}O_4$	Decreased	Increased	Constant	ES	$C_{12}H_{11}O_4Cl$
$C_{13}H_{10}O_5$	Decreased	Increased	Constant	ES	$C_{13}H_9O_5Cl$
$C_{11}H_6O_7$	Increased	Increased	Constant	ES	$C_{11}H_5O_7Cl$
$C_{12}H_{10}O_6$	Constant	Increased	Constant	ES	$C_{12}H_9O_6Cl$
$C_8H_{14}O_9$	Newly Formed	Increased	Constant	ES	$C_8H_{13}O_9Cl$
$C_{10}H_{10}O_6$	Decreased	Increased	Constant	ES	$C_{10}H_9O_6Cl$
$C_{13}H_{12}O_6$	Decreased	Increased	Constant	ES	$C_{13}H_{11}O_6Cl$
$C_{12}H_{18}O_7$	Disappeared	Newly Formed	Constant	ES	$C_{12}H_{17}O_7Cl$
$C_{18}H_{12}O_3$	Disappeared	Newly Formed	Increased	ES	$C_{18}H_{11}O_3Cl$
$C_{15}H_{24}O_5$	Newly Formed	Disappeared	Newly Formed	ES	$C_{15}H_{23}O_5Cl$
$C_{11}H_{10}O_7$	Constant	Increased	Constant	ES	$C_{11}H_8O_7Cl_2$
$C_{12}H_{18}O_8$	Disappeared	Newly Formed	Constant	ES	$C_{12}H_{17}O_8Cl$
$C_{14}H_{24}O_7$	Constant	Constant	Increased	ES	$C_{14}H_{23}O_7Cl$
$C_{12}H_{26}O_9$	Constant	Decreased	Decreased	ES	$C_{12}H_{25}O_9Cl$
$C_{16}H_{32}O_3$	Decreased	Increased	Constant	ES	$C_{16}H_{30}O_3Cl_2$
$C_{16}H_{24}O_8$	Newly Formed	Disappeared	ND	ES	$C_{16}H_{23}O_8Cl$
$C_{19}H_{26}O_6$	Newly Formed	Disappeared	ND	ES	$C_{19}H_{25}O_6Cl$
$C_{18}H_{32}O_3$	Constant	Constant	Constant	ES	$C_{18}H_{29}O_3Cl_3$
$C_{19}H_{28}O_7$	Decreased	Increased	Decreased	ES	$C_{19}H_{27}O_7Cl$
$C_{12}H_{12}O_7$	Decreased	Increased	Increased	ES	$C_{12}H_{11}O_7Cl$
$C_{12}H_{14}O_7$	Decreased	Increased	Constant	ES	$C_{12}H_{13}O_7Cl$
$C_{14}H_{22}O_5$	Decreased	Increased	Constant	ES	$C_{14}H_{21}O_5Cl$
$C_{11}H_{10}O_6$	Decreased	Increased	Constant	ES	$C_{11}H_8O_6Cl_2$
$C_{11}H_{12}O_8$	Disappeared	Newly Formed	Constant	ES	$C_{11}H_{11}O_8Cl$
$C_{10}H_{10}O_7$	Decreased	Constant	Constant	ES	$C_{10}H_9O_7Cl$
$C_{13}H_{14}O_7$	Decreased	Increased	Constant	ES	$C_{13}H_{13}O_7Cl$
$C_{13}H_{26}O_2$	Disappeared	Newly Formed	Constant	ES	$C_{13}H_{23}O_2Cl_3$
$C_{13}H_{16}O_7$	Decreased	Increased	Constant	ES	$C_{13}H_{15}O_7Cl$
$C_{12}H_{16}O_8$	Decreased	Increased	Constant	ES	$C_{12}H_{15}O_8Cl$
$C_{14}H_{24}O_2$	Decreased	Increased	Constant	ES	$C_{14}H_{23}O_2Cl$
$C_{12}H_{10}O_9$	ND	Newly Formed	Increased	ES	$C_{12}H_9O_9Cl$
$C_{12}H_{26}O_8$	Constant	Constant	Constant	ES	$C_{12}H_{25}O_8Cl$
$C_{14}H_{16}O_8$	Decreased	Increased	Constant	ES	$C_{14}H_{15}O_8Cl$
$C_{15}H_{20}O_7$	Decreased	Increased	Constant	ES	$C_{15}H_{19}O_7Cl$

Precursors	Changes in intensities between two consecutive processes			Formation mechanism	DBPs
	RW→CW	CW→FW	FW→Finished water		
$C_{15}H_{14}O_8$	Decreased	Increased	Constant	ES	$C_{15}H_{13}O_8Cl$
$C_{17}H_{26}O_6$	Decreased	Constant	Constant	ES	$C_{17}H_{25}O_6Cl$
$C_{15}H_{20}O_8$	Decreased	Constant	Constant	ES	$C_{15}H_{19}O_8Cl$
$C_{14}H_{16}O_7$	Decreased	Increased	Constant	ES	$C_{14}H_{14}O_7Cl_2$
$C_{17}H_{18}O_7$	Disappeared	Newly Formed	Constant	ES	$C_{17}H_{17}O_7Cl$
$C_{20}H_{30}O_6$	Decreased	Increased	Constant	ES	$C_{20}H_{29}O_6Cl$
$C_{17}H_{22}O_7$	Decreased	Constant	Constant	ES	$C_{17}H_{20}O_7Cl_2$
$C_{16}H_{18}O_9$	Disappeared	Newly Formed	Constant	ES	$C_{16}H_{16}O_9Cl_2$
$C_{18}H_{24}O_{10}$	Decreased	Decreased	Constant	ES	$C_{18}H_{23}O_{10}Cl$
$C_{16}H_{22}O_5$	Disappeared	ND	Newly Formed	ES	$C_{16}H_{21}O_5Cl$
$C_{15}H_{22}O_4$	Decreased	Constant	Constant	ES	$C_{15}H_{21}O_4Cl$
$C_{12}H_{14}O_9$	Decreased	Constant	Constant	ES	$C_{12}H_{13}O_9Cl$
$C_{14}H_{20}O_4$	Decreased	Constant	Constant	ES	$C_{14}H_{19}O_4Cl$
$C_{17}H_{22}O_6$	Decreased	Constant	Decreased	ES	$C_{17}H_{21}O_6Cl$
$C_{12}H_{16}O_7$	Decreased	Increased	Increased	ES	$C_{12}H_{14}O_7Cl_2$
$C_{16}H_{20}O_6$	Decreased	Constant	Increased	ES	$C_{16}H_{19}O_6Cl$
$C_{17}H_{28}O_5$	Decreased	Increased	Constant	ES	$C_{17}H_{27}O_5Cl$
$C_9H_6O_3$	Constant	Increased	Constant	AR	$C_9H_7O_4Cl$
$C_{12}H_{10}O_3$	Decreased	Increased	Constant	AR	$C_{12}H_{11}O_4Cl$
$C_9H_4O_6$	Constant	Increased	Constant	AR	$C_9H_5O_7Cl$
$C_{12}H_8O_5$	Constant	Increased	Constant	AR	$C_{12}H_9O_6Cl$
$C_{13}H_{10}O_5$	Decreased	Increased	Constant	AR	$C_{13}H_{11}O_6Cl$
$C_{12}H_{16}O_6$	Disappeared	Newly Formed	Constant	AR	$C_{12}H_{17}O_7Cl$
$C_{15}H_{22}O_4$	Newly Formed	Disappeared	Newly Formed	AR	$C_{15}H_{23}O_5Cl$
$C_{12}H_{16}O_7$	Disappeared	Newly Formed	Constant	AR	$C_{12}H_{17}O_8Cl$
$C_{14}H_{20}O_6$	Newly Formed	Disappeared	Newly Formed	AR	$C_{14}H_{21}O_7Cl$
$C_{14}H_{22}O_6$	Constant	Constant	Increased	AR	$C_{14}H_{23}O_7Cl$
$C_{17}H_{24}O_5$	Decreased	Constant	Constant	AR	$C_{17}H_{25}O_6Cl$
$C_{18}H_{28}O_7$	Newly Formed	Disappeared	ND	AR	$C_{18}H_{29}O_8Cl$
$C_{10}H_8O_5$	Decreased	Increased	Constant	AR	$C_{10}H_9O_6Cl$
$C_{11}H_{18}O_5$	Constant	Disappeared	ND	AR	$C_{11}H_{19}O_6Cl$
$C_{12}H_{10}O_5$	Decreased	Increased	Constant	AR	$C_{12}H_{11}O_6Cl$
$C_{11}H_{10}O_6$	Decreased	Increased	Constant	AR	$C_{11}H_{11}O_7Cl$
$C_{16}H_{16}O_2$	Decreased	Increased	Disappeared	AR	$C_{16}H_{17}O_3Cl$
$C_{12}H_{10}O_6$	Decreased	Increased	Increased	AR	$C_{12}H_{11}O_7Cl$
$C_{12}H_{12}O_6$	Decreased	Increased	Constant	AR	$C_{12}H_{13}O_7Cl$
$C_{14}H_{20}O_4$	Decreased	Increased	Constant	AR	$C_{14}H_{21}O_5Cl$
$C_{11}H_{10}O_7$	Disappeared	Newly Formed	Constant	AR	$C_{11}H_{11}O_8Cl$
$C_{10}H_6O_5$	Constant	Increased	Constant	AR	$C_{10}H_7O_6Cl$

Precursors	Changes in intensities between two consecutive processes			Formation mechanism	DBPs
	RW→CW	CW→FW	FW→Finished water		
$C_{12}H_{22}O_6$	Decreased	Increased	Constant	AR	$C_{12}H_{23}O_7Cl$
$C_{13}H_{12}O_6$	Decreased	Increased	Constant	AR	$C_{13}H_{13}O_7Cl$
$C_{13}H_{14}O_6$	Decreased	Increased	Constant	AR	$C_{13}H_{15}O_7Cl$
$C_{12}H_{14}O_7$	Decreased	Increased	Constant	AR	$C_{12}H_{15}O_8Cl$
$C_{14}H_{14}O_7$	Decreased	Increased	Constant	AR	$C_{14}H_{15}O_8Cl$
$C_{15}H_{18}O_6$	Decreased	Increased	Constant	AR	$C_{15}H_{19}O_7Cl$
$C_{12}H_8O_6$	Constant	Increased	Constant	AR	$C_{12}H_{10}O_8Cl_2$
$C_{13}H_{12}O_5$	Decreased	Increased	Constant	AR	$C_{13}H_{14}O_7Cl_2$
$C_{15}H_{18}O_7$	Decreased	Constant	Constant	AR	$C_{15}H_{19}O_8Cl$
$C_{17}H_{16}O_6$	Disappeared	Newly Formed	Constant	AR	$C_{17}H_{17}O_7Cl$
$C_{20}H_{28}O_5$	Decreased	Increased	Constant	AR	$C_{20}H_{29}O_6Cl$
$C_{16}H_{14}O_7$	Disappeared	Newly Formed	Constant	AR	$C_{16}H_{16}O_9Cl_2$
$C_{18}H_{22}O_9$	Decreased	Decreased	Constant	AR	$C_{18}H_{23}O_{10}Cl$
$C_{12}H_{12}O_8$	Decreased	Constant	Constant	AR	$C_{12}H_{13}O_9Cl$
$C_{11}H_{12}O_9$	ND	Newly Formed	Constant	AR	$C_{11}H_{13}O_{10}Cl$
$C_{18}H_{24}O_3$	Decreased	Constant	Decreased	AR	$C_{18}H_{25}O_4Cl$
$C_{12}H_{12}O_5$	Decreased	Increased	Constant	AR	$C_{12}H_{13}O_6Cl$
$C_{16}H_{18}O_5$	Decreased	Constant	Increased	AR	$C_{16}H_{19}O_6Cl$

*ES – electrophilic substitution, AR – addition reaction, ND – not detected

Table S7 Complete list of CHON precursors and their fates during water treatment processes

Precursors	Changes in intensities between two consecutive processes			DBPs
	RW→CW	CW→FW	FW→Finished water	
$C_6H_{10}ON_2$	Decreased	Increased	Increased	$C_6H_7ON_2Cl_3$
$C_8H_7O_4N$	Disappeared	Newly Formed	Constant	$C_8H_5O_4NCl_2$
$C_9H_{14}O_3N_2$	Decreased	Increased	Constant	$C_9H_{13}O_3N_2Cl$
$C_{12}H_{12}O_2N_2$	Constant	Constant	Decreased	$C_{12}H_{11}O_2N_2Cl$
$C_{11}H_8O_3N_2$	Decreased	Increased	Constant	$C_{11}H_7O_3N_2Cl$
$C_{12}H_{16}O_4N_2$	Disappeared	Newly Formed	Decreased	$C_{12}H_{13}O_4N_2Cl_3$
$C_{19}H_{26}O_3N_2$	Decreased	Constant	Constant	$C_{19}H_{25}O_3N_2Cl$
$C_{16}H_{22}O_2N_2$	Decreased	Constant	Constant	$C_{16}H_{21}O_2N_2Cl$
$C_{15}H_{22}O_3N_2$	Decreased	Constant	Constant	$C_{15}H_{21}O_3N_2Cl$
$C_{21}H_{20}O_3N_2$	Decreased	Constant	Constant	$C_{21}H_{18}O_3N_2Cl_2$
$C_{22}H_{22}O_3N_2$	Disappeared	ND	Newly Formed	$C_{22}H_{21}O_3N_2Cl$
$C_{15}H_{32}O_{11}N_2$	Constant	Disappeared	Newly Formed	$C_{15}H_{31}O_{11}N_2Cl$
$C_{21}H_{27}O_{10}N$	Decreased	Increased	Constant	$C_{21}H_{26}O_{10}NCl$
$C_{16}H_{22}O_2N_2$	Decreased	Constant	Constant	$C_{16}H_{21}O_2N_2Cl$
$C_{10}H_{20}O_8N_2$	Constant	Constant	Constant	$C_{10}H_{19}O_8N_2Cl$
$C_{12}H_{23}O_3N$	Decreased	Constant	Constant	$C_{12}H_{20}O_3NCl_3$
$C_{17}H_{22}O_3N_2$	Decreased	Constant	Constant	$C_{17}H_{21}O_3N_2Cl$
$C_{17}H_{22}O_4N_2$	Decreased	Constant	Constant	$C_{17}H_{21}O_4N_2Cl$
$C_{19}H_{30}O_2N_2$	Newly Formed	Disappeared	ND	$C_{19}H_{29}O_2N_2Cl$
$C_{19}H_{26}O_3N_2$	Decreased	Constant	Constant	$C_{19}H_{25}O_3N_2Cl$
$C_{16}H_{22}O_6N_2$	Decreased	Increased	Increased	$C_{16}H_{21}O_6N_2Cl$
$C_{16}H_{22}O_2N_2$	Decreased	Constant	Constant	$C_{16}H_{21}O_2N_2Cl$
$C_{16}H_{12}O_7N_2$	Decreased	Disappeared	Newly Formed	$C_{16}H_{11}O_7N_2Cl$
$C_{15}H_{22}O_3N_2$	Decreased	Constant	Constant	$C_{15}H_{21}O_3N_2Cl$
$C_{19}H_{30}O_2N_2$	Newly Formed	Disappeared	ND	$C_{19}H_{29}O_2N_2Cl$
$C_{17}H_{12}O_7N_2$	Decreased	Constant	Constant	$C_{17}H_{11}O_7N_2Cl$
$C_{21}H_{20}O_3N_2$	Decreased	Constant	Constant	$C_{21}H_{18}O_3N_2Cl_2$
$C_{17}H_{18}O_9N_2$	Newly Formed	Disappeared	ND	$C_{17}H_{17}O_9N_2Cl$
$C_{21}H_{28}O_6N_2$	Decreased	Constant	Constant	$C_{21}H_{27}O_6N_2Cl$
$C_{15}H_{32}O_{11}N_2$	Constant	Disappeared	Newly Formed	$C_{15}H_{31}O_{11}N_2Cl$
$C_{21}H_{27}O_{10}N$	Decreased	Increased	Constant	$C_{21}H_{26}O_{10}NCl$
$C_{17}H_{18}O_3N_2$	Constant	Increased	Increased	$C_{17}H_{17}O_3N_2Cl$
$C_{16}H_{18}O_4N_2$	ND	Newly Formed	Constant	$C_{16}H_{17}O_4N_2Cl$
$C_{15}H_{22}O_3N_2$	Decreased	Constant	Constant	$C_{15}H_{21}O_3N_2Cl$
$C_{21}H_{24}O_3N_2$	Decreased	Increased	Increased	$C_{21}H_{23}O_3N_2Cl$
$C_{17}H_{10}O_8N_2$	Disappeared	Newly Formed	Increased	$C_{17}H_9O_8N_2Cl$
$C_{21}H_{27}O_{10}N$	Decreased	Increased	Constant	$C_{21}H_{26}O_{10}NCl$
$C_{12}H_{10}O_4N_2$	Decreased	Increased	Constant	$C_{12}H_9O_4N_2Cl$

Precursors	Changes in intensities between two consecutive processes			DBPs
	RW→CW	CW→FW	FW→Finished water	
$C_{17}H_{20}O_4N_2$	Decreased	Increased	Constant	$C_{17}H_{19}O_4N_2Cl$
$C_{14}H_{23}O_7N$	ND	Newly Formed	Increased	$C_{14}H_{22}O_7NCl$

*ND – not detected