Supplementary Material

Unraveling the chemodiversity of halogenated disinfection by-products formed during drinking water treatment using target and non-target screening tools

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I. Targeted disinfection byproducts

Table S1. Target DBPs, and corresponding acronyms, CAS numbers, purity and provider of the analytical standard, molecular formula, and mass.

DBP class	Analyte	Acronym	Molecular formula	Mass (Da)*	CAS Number	Supplier (purity, %)
Trihalo-methanes (THMs)	Dibromochloromethane	DBCM	Br_2ClCH	206	124-48-1	Sigma (>99)
	Bromoform	TBM	Br_3CH	250	75-25-2	Sigma (>99)
	Dichloro-iodomethane	DCIM	Cl_2ICH	210	594-04-7	CanSyn (>95)
	Chloro-bromo-iodomethane	BCIM	$BrClICH$	254	34970-00-8	CanSyn (>95)
	Dibromo-iodomethane	DBIM	Br_2ICH	298	593-94-2	CanSyn (90-95)
	Chloro-diiodomethane	CDIM	ClI_2CH	302	638-73-3	CanSyn (90-95)
	Bromo-diiodomethane	BDIM	BrI_2CH	346	557-95-9	CanSyn (90-95)
	Iodoform	TIM	I_3CH	394	75-47-8	Sigma (99)
Trihalo-acetal-dehydes (THALs)	Chloral	TCAL	Cl_3C_2HO	146	75-87-6	Sigma (>98)
	Bromodichloroacetaldehyde	BDCAL	$BrCl_2C_2HO$	190	34619-29-9	CanSyn (90-95)
	Dibromochloroacetaldehyde	DBCAL	Br_2ClC_2HO	234	64316-11-6	CanSyn (90-95)
	Bromal	TBAL	Br_3C_2HO	278	115-17-3	Sigma (>97)
Halo-aceto-nitriles (HANs)	Chloroacetonitrile	CAN	C_2H_2ClN	75	107-14-2	Sigma (>99)
	Bromoacetonitrile	BAN	C_2H_2BrN	119	590-17-0	Sigma (>97)
	Iodoacetonitrile	IAN	C_2H_2IN	167	624-75-9	Sigma (>98)
	Dichloroacetonitrile	DCAN	C_2HCl_2N	109	3018-12-0	Sigma (>98)
	Dibromoacetonitrile	DBAN	C_2HBr_2N	197	3252-43-5	Sigma (>90)
	Bromodichloroacetonitrile	BDCAN	C_2BrCl_2N	187	60523-73-1	CanSyn (>85)
	Dibromochloroacetonitrile	DBCAN	C_2Br_2ClN	231	144772-39-4	CanSyn (>85)
	Tribromoacetonitrile	TBAN	C_2Br_3N	275	75519-19-6	CanSyn (90-95)
Halo-acetamides (HACMs)	Chloroacetamide	CACM	ClC_2H_4ON	93	79-07-2	Sigma (>98)
	Bromoacetamide	BACM	BrC_2H_4ON	137	683-57-8	Sigma (>98)
	Iodoacetamide	IACM	IC_2H_4ON	185	144-48-9	Sigma (>98)
	Bromochloroacetamide	BCACM	$BrClC_2H_3ON$	171	62872-24-8	CanSyn (>99)
	Dichloroacetamide	DCACM	$Cl_2C_2H_3ON$	127	683-72-7	Sigma (>99)
	Dibromoacetamide	DBACM	$Br_2C_2H_3ON$	215	598-70-9	CanSyn (>99)
	Chloroiodoacetamide	CIACM	$ClIC_2H_3ON$	219	62872-35-9	CanSyn (>99)
	Bromoiodoacetamide	BIACM	$BrIC_2H_3ON$	263	62872-36-0	CanSyn (>85)
	Diiodoacetamide	DIACM	$I_2C_2H_3ON$	311	5875-23-0	CanSyn (>99)
	Trichloroacetamide	TCACM	$Cl_3C_2H_2ON$	161	594-65-0	Sigma (>99)
	Bromodichloroacetamide	BDCACM	$BrCl_2C_2H_2ON$	205	98137-00-9	CanSyn (>99)
	Dibromochloroacetamide	DBCACM	$ClBr_2C_2H_2ON$	249	855878-13-6	CanSyn (>99)
	Tribromoacetamide	TBACM	$Br_3C_2H_2ON$	293	594-47-8	CanSyn (>99)
Haloacids (HAAs)	Chloroacetic acid	CAA	$ClC_2H_3O_2$	94	79-11-8	Sigma (>99)
	Bromoacetic acid	BAA	$BrC_2H_3O_2$	138	79-08-3	Sigma (>99)
	Iodo acetic acid	IAA	$IC_2H_3O_2$	186	64-69-7	Sigma (98)
	Chlorobromo acetic acid	BCAA	$BrClC_2H_2O_2$	172	5589-96-8	Sigma (>99)
	Dichloroacetic acid	DCAA	$Cl_2C_2H_2O_2$	128	79-53-6	Sigma (>99)
	Dibromoacetic acid	DBAA	$Br_2C_2H_2O_2$	216	631-64-1	Sigma (>99)
	Chloroiodoacetic acid	CIAA	$ClIC_2H_2O_2$	220	53715-09-6	CanSyn (>90)
	Bromoiodoacetic acid	BIAA	$BrIC_2H_2O_2$	264	71815-43-5	CanSyn (>85)
	Diiodoacetic acid	DIAA	$l_2C_2H_2O_2$	312	598-89-00	CanSyn (>90)
	Trichloroacetic acid	TCAA	$Cl_3C_2HO_2$	162	76-03-9	Sigma (>99)
	Bromodichloroacetic acid	BDCAA	$BrCl_2C_2HO_2$	206	71133-14-7	Sigma (>99)
	Dibromochloroacetic acid	DBCAA	$Br_2ClC_2HO_2$	250	5278-95-5	Sigma (>99)
	Tribromoacetic acid	TBAA	$Br_3C_2HO_2$	294	75-96-7	Sigma (>99)
	Dalapon (2,2-dichloropropanoic acid)	DCPA	$Cl_2C_3H_4O_2$	142	75-99-0	Sigma (>99)

*Nominal monoisotopic mass (Da).

II. Chemicals and reagents

Ultrapure water (resistivity of 18.2 MΩ·cm at 25 °C; TOC ≤ 5 ppb) used to prepare analytical methods blanks and to rinse sampling bottles and labware during the cleaning process was obtained using a Milli-Q Advantage system and aQ-POD dispenser equipped with a Millipack® Express 40 filter (Asymmetric PolyEtherSulfone (PES) membrane, 0.22 µm) for particles and bacteria removal, connected in series with a LC-Pack® Point-of-use Polisher cartridge (C18 reverse-phase silica) for trace organics removal (Merck Millipore).

All reagents and solvents used were of high purity and mostly supplied either by VWR International (Spånga, Sweden) or Merck KgaA (Darmstadt, Germany).

L(+)-ascorbic acid and sodium thiosulfate pentahydrate used to quench chlorine in water were Normapur® grade and supplied by VWR. Anhydrous sodium sulfate used to increase the ionic strength of the water to improve LLE efficiency and to dry the extracts was also Normapur® grade (VWR). ISOLUTE® Na_2SO_4 drying cartridges used to dry extracts for HACMs and HAAs analysis were obtained from Biotage, Sweden.

As for the acids used, ACS reagent grade formic acid (98-100%) (Emsure®), nitric acid 70%, and hydrochloric acid 30% (Suprapure®) were provided by Merck, whereas sulfuric acid 96% was supplied by VWR.

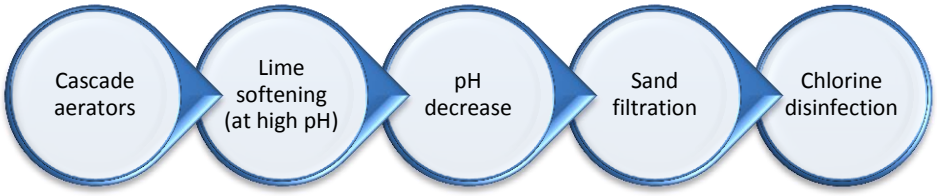
The solvents used for sample extraction and liquid chromatography analysis were: Ethyl acetate (EtAc) for pesticide residue analysis, HPLC-grade water (Chromasolv^{TM}), and HPLC-grade methanol (MeOH) (LiChrosolv®) and methyl *tert*-butyl ether (MTBE) (SupraSolv®) were provided by Merck.

All reagents used in the production of diazomethane (derivatization agent) were supplied by Sigma Aldrich (Merck): diazald® (99%), Aldrich® diazomethane-generator with System 45^{TM} compatible connection, diethylene glycol monoethyl ether (carbitol ^{TM}) (99%) and ACS-grade potassium hydroxide.

III. Water treatment in the investigated drinking water treatment plants (DWPTs)

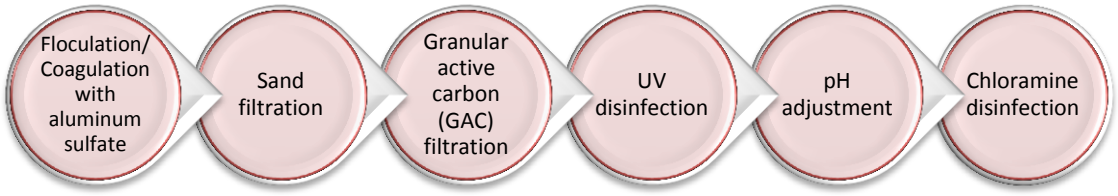
DWTP1 (46,000 m^3/day)

Artificial groundwater (surface water infiltrated into the subsoil)



DWTP2 (200,000 m^3/day)

Surface water



DWTP3 (26,000 m^3/day)

Groundwater

DWTP4 (10,000 m^3/day)

Surface water

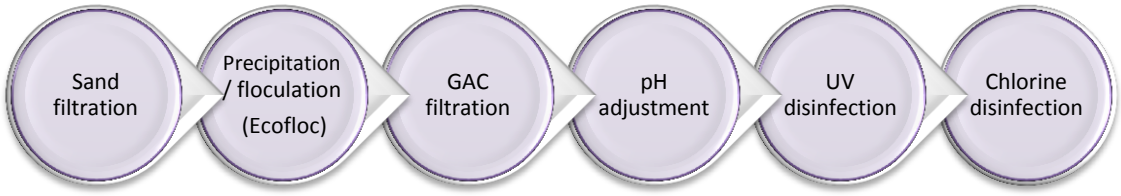


Figure S1. Scheme of the water treatment trains implemented in the DWTPs investigated**.**

IV. Additional physical-chemical characterization of water samples

Table S2. Additional physical-chemical characterization of water samples.

SAMPLE CODE	A_{254} (Abs/m)	Cl^- (mg/L)	$S\text{-}SO_4^-$ (mg/L)	F^- (mg/L)	$I\text{-}IO_3^-$ (mg/L)	$N\text{-}NH_4^+$ (mg/L)	$N\text{-}NO_2^-$ (mg N/L)	$N\text{-}NO_3^-$ (mg N/L)	Na^+ (mg/L)	K^+ (mg/L)	Mg^{2+} (mg/L)	Ca^{2+} (mg/L)
LOQs	-	*0.03*	*0.02*	*0.01*	*0.03*	*0.01*	*0.004*	*0.02*	*0.01*	*0.01*	*0.01*	*0.5*
DWTP1 IN	7.3	35	11	0.77	5.6	<LOQ	<LOQ	1.9	16	5.0	10	32
DWTP1 OUT	6.6	35	11	0.77	5.6	<LOQ	<LOQ	1.9	16	5.1	10	33
DWTP2 IN	7.3	15	15.	0.15	1.1	<LOQ	<LOQ	0.04	13	2.7	4.7	24
DWTP2 OUT	6.9	15	15.	0.16	1.1	0.06	0.01	0.04	13	2.7	4.7	31
DWTP3 IN	4.9	55	5.2	0.29	2.1	<LOQ	<LOQ	1.1	36	2.9	15	15
DWTP3 OUT	4.8	556	5.2	0.29	2.1	0.02	0.06	1.1	36	2.9	15	15
DWTP4 IN	5.6	18	3.2	0.19	1.4	<LOQ	<LOQ	0.02	13	1.7	2.5	17
DWTP4 OUT	4.8	19	3.1	0.19	1.3	<LOQ	<LOQ	0.03	16	1.7	2.5	18

*measured in the sample collected before disinfection; **measured in the sample collected after disinfection.

Iodide (I^-), and phosphate ($P\text{-}PO_4^{-3}$), chlorite (ClO_2^-) and chlorate (ClO_3^-) were <LOQ in all samples (LOQ of I^-: 0.025 mg/L, LOQ of $P\text{-}PO_4^{-3}$: 0.003 mg/L, LOQ of ClO_2^-: 0.005 mg/L and LOQ of ClO_3^-: 0.011 mg/L.

V. Target DBP analysis

- ***Sample extraction***

The LLE approaches used to extract targeted DBPs from water samples were based on the US Environmental Protection Agency (USEPA) method for the analysis of DBPs in drinking water (Hodgeson and Cohen 1990). All samples were extracted in duplicate.

Ascorbic acid (2.5 mg/L) freshly prepared in Milli-Q-grade water was used to quench residual free chlorine (<0.5 mg/L) in the samples and preserve the target DBPs.

For extraction of THMs, THALs, and THANs, 100 mL of water was acidified to pH<0.5 with 5 mL of concentrated H_2SO_4 and then 30 g of dried granular Na_2SO_4 was added to increase the ionic strength of the water and favor the partition of the analytes into the extracting solvent (MTBE). After dissolution, the internal standard (IS) (100 µL x 1 µg/mL of 1,2-dibromopropane (Sigma Aldrich) in MTBE) was added and mixed in the solution. Finally, the extracting solvent (2.5 mL of MTBE) was added. Samples were agitated with a mechanical shaker at 500 rpm for 30 min. After settling for 5 min, the MTBE, laying on the top of the sample, was collected and dried using a Na_2SO_4 column, and stored in a 2-mL vial at -20ºC in the dark until GC-MS analysis.

To extract HAAs, a similar procedure was followed, using 50 mL and proportional amounts of H_2SO_4 (2.5 mL) and Na_2SO_4 (15 g). After dissolution, the internal standard (IS) (100 µL x 1 µg/mL of 2.,3-dibromopropanoic acid (Sigma Aldrich) in MTBE). Then, 5 mL of the extracting solvent (MTBE) was added and the sample was vigorously manually shaken for 2 min. After settling for 5 min, the MTBE, laying on the top of the sample, was collected and transferred to 20 mL vial. The extraction step with 5 mL of MTBE was repeated twice, and finally, the combined MTBE extract was dried using ISOLUTE® Na_2SO_4 drying cartridges (Biotage, Sweden) and concentrated under N_2 to a volume of 0.4 mL in a graduated test tube. The HAA extract (0.4 mL) was derivatized for one hour at room temperature with 0.2 mL of freshly prepared diazomethane. During the derivatization process, the methyl esters of HAAs were formed. These compounds are more volatile than HAAs and thus, amenable to GC-MS analysis. Diazomethane was produced in small (~3 mL) amounts from diazald using a diazomethane generator (Sigma Aldrich, Merck), following the

manufacturer indications. After derivatization, the extract was transferred to a 2-mL vial with 300 µL insert for GC-MS analysis.

The extraction of HACMs was conducted following the same steps as aforementioned for the extraction of HAAs. However, three main differences in the extraction protocol have to be highlighted: i) the water pH was lowered only to 5 with diluted H_2SO_4 to avoid HACMs degradation, ii) the use of ^{13}C-bromoacetamide dissolved in EtAc as IS, and iii) the use of EtAc as extracting solvent. The combined extract of EtAc obtained after three extraction cycles was dried using ISOLUTE® Na_2SO_4 drying cartridges and concentrated under N_2 to a volume of 0.2 mL in a graduated test tube. Finally, the concentrated extract was transferred to a 2-mL vial with 300 µL insert for GC-MS analysis.

- ***GC-EI-MS analysis of THMs, THALs, HANs, and HACMs***

Analytical determination of THMs, THALs, HANs, and HACMs in MTBE extracts was performed using a 7890B GC connected in series to a 5977A MSD (Agilent Technologies). One µL of the extract was injected in splitless mode using a 7693 automated autosampler equipped with a multimode inlet (split flow=50 mL/min, splitless time=1.5 min). The temperature of the injector was maintained at 200ºC for 0.1 s and rapidly increased to 300 ºC (600ºC/min). GC separation was achieved with a capillary GC column Rtx-200 MS (30 m x 0.25 mm x 0.25 µm) (Restek, Teknokroma, Barcelona), 1.2 mL/min of constant Helium flow, and a temperature gradient. For the analysis of THMs, THALs, and HANs the temperature gradient started at 30ºC (held for 5 min), and ramped at a rate of 9ºC/min to 165 ºC, and then at a rate of 20 ºC/min to 300ºC (held for 5 min). In the case of HACMs, the temperature gradient started at 50ºC (held for 3 min) and then, ramped at a rate of 9ºC/min to 165ºC and a rate of 25ºC/min to 285 ºC (held for 10 min). During both analytical runs, the temperatures of the GC-MS transfer line, and the MS source were set to 280 ºC and 200 ºC, respectively.

The analyzer was operated in selected ion monitoring (SIM) mode. A minimum of four ions was registered per analyte (see Table S3). Figures S2 and S3 show the total ion chromatogram obtained after analysis of calibration standard solutions at a concentration of 10 µg/mL. Mass acquisition and data analysis were performed using Mass Hunter B.07.00 software (Agilent Technologies).

The THMs chloroform (TCM) and dichlorobromomethane (DCBM) were not captured with the analytical conditions used as they eluted in the solvent peak front and therefore, they had to be excluded from the analysis.

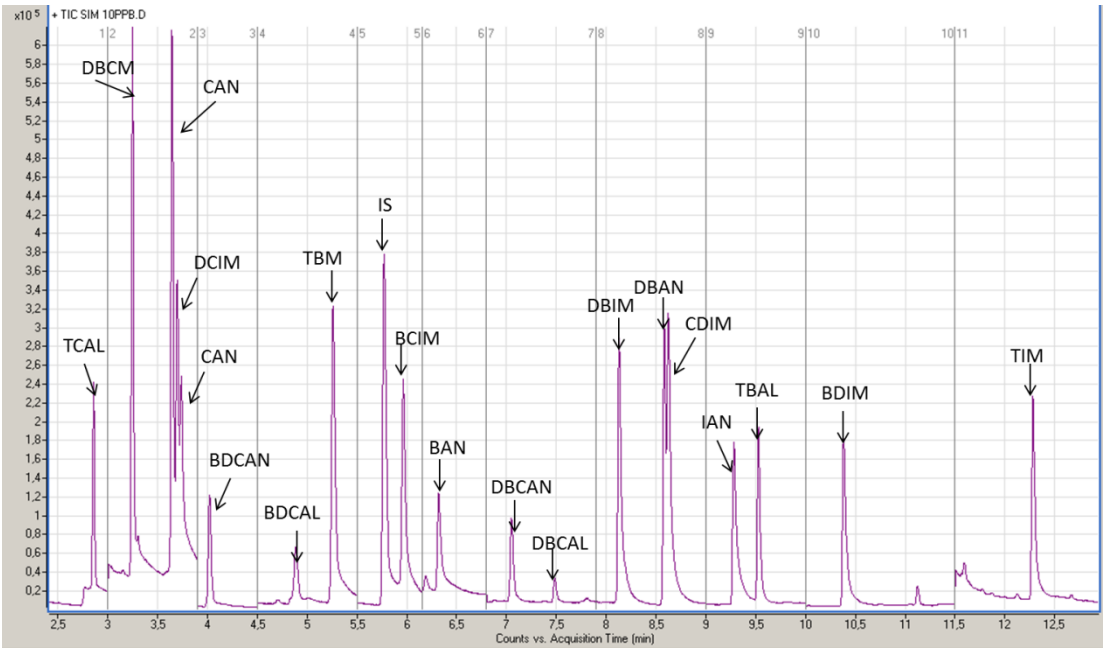


Figure S2. Total ion chromatogram (TIC) obtained after GC-EI-MS analysis of MilliQ water fortified with the target THMs, THALs, and HANs at a concentration of 10 µg/L.

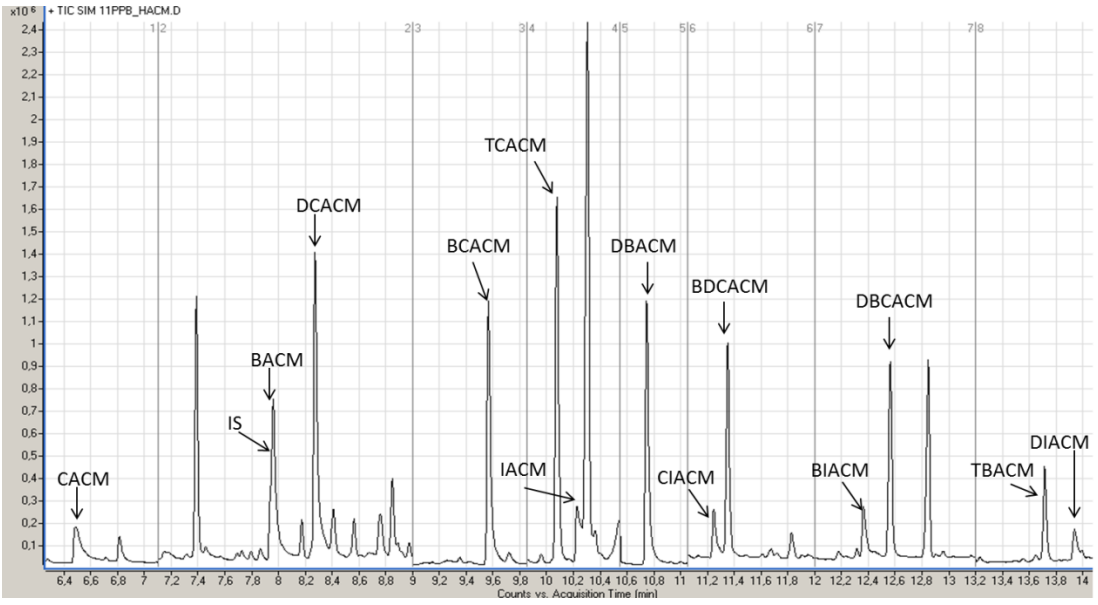


Figure S3. Total ion chromatogram (TIC) obtained after GC-EI-MS analysis of MilliQ water fortified with the target HACMs at a concentration of 10 µg/L.

- **GC-EI-MS/MS analysis of HAAs.**

Analytical determination of methyl esters of HAAs was performed using a 7890B GC connected in series to a 7000C triple quadrupole (Agilent Technologies). Ionization was carried out in the electron ionization mode. One µL of the derivatized extract was injected in splitless mode using a7638B automated injector (split flow=50 mL/min, splitless time=1.5 min). GC separation of the analytes was achieved using a capillary GC column Rtx-200 MS (30 m x 0.25 mm x 0.25 µm) (Restek, Teknokroma, Barcelona), 1.2 mL/min constant flow of Helium and a temperature gradient (40 ºC held for 2 min, then increased at 10 ºC/min to 65 ºC and held for 2 min, and further increased at 10 ºC/min to 110ºC and at 20ºC/min to 285 ºC and held for 15 min. The temperatures of the injector, the GC/MS transfer line, and the MS source were set to 250 ºC, 280 ºC, and 200 ºC, respectively.

The analyzer was operated in selected reaction monitoring (SRM) mode, using nitrogen (1.5 mL/min) as the collision gas. A minimum of two SRM transitions was acquired per analyte (see Table S3). Figure S4 shows the total ion chromatogram obtained after the analysis of a standard calibration solution at a concentration of 10 µg/mL. Mass acquisition was performed using MSD ChemStation and data analysis was done with Mass Hunter B.08 (Agilent Technologies).

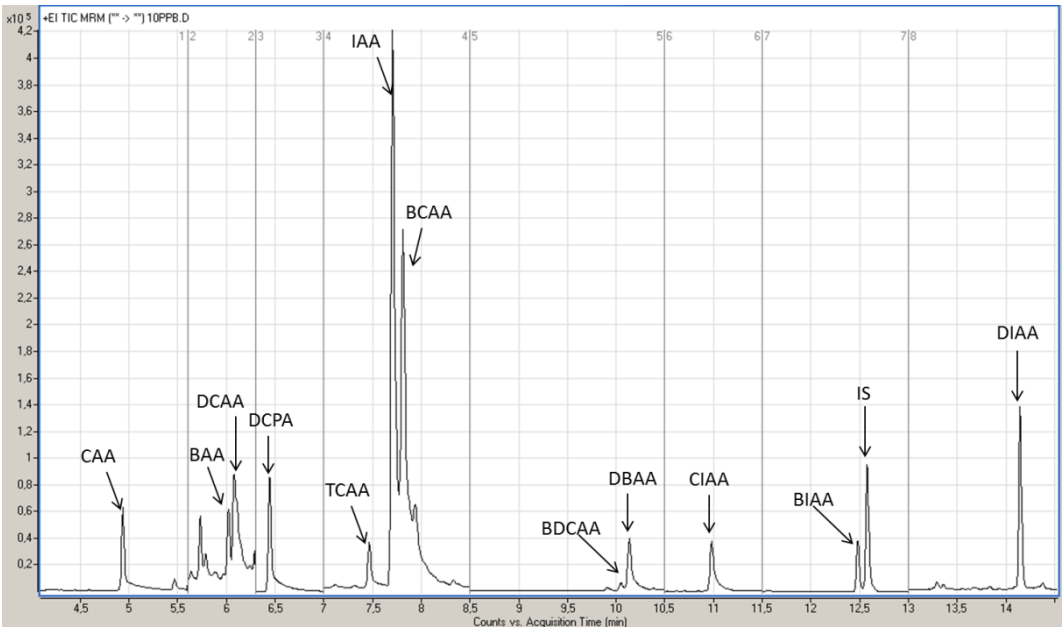


Figure S4. Total ion chromatogram (TIC) obtained after GC-EI-MS/MS analysis of MilliQ water fortified with the target HAAs at a concentration of 10 µg/L.

- ***Performance of target methods***

The performance of the targeted methods was evaluated in terms of linearity, sensitivity, and accuracy (analyte recovery) and method repeatability. The results are summarized in Table S3.

Quantification was performed by the internal standard method. For this, calibration curves were constructed by plotting the ratio of the analyte and the internal standard peak areas obtained in the different standard calibration solutions (Milli Q water fortified at different concentration levels with the mixture of the target DBPs). A minimum of five calibration data points (exceptionally four in the case of few DBPs) in the range 0.1-50 µg/L in the case of THMs, THALs, and HANs, and 0.05-50 µg/L in the case of HACMs, and HAAs were used to construct these calibration curves. Quantitation of each analyte in the investigated samples was done according to the least-squares linear regression model obtained after the linear fitting of its calibration curve. The linearity range observed for each analyte and the coefficient of determination obtained for the corresponding model are summarized in Table S3.

Method sensitivity was estimated from the analyte signal observed at the lowest calibration solutions. Method reporting limits corresponded with the analyte concentration that provided a signal-to-noise ratio of 10, and concentrations below the MRL with an S/N ratio of 3 were provided as detected but could not be quantified.

Analyte absolute recoveries and method repeatability were evaluated through a recovery study. For this, LC-grade waters were fortified with the target DBPs at 0.5 µg/L (n=4) or higher concentration in the case of regulated THMs, DBCM, and TBM, and the trihalo-HANs BDCAN, DBCAN and TBAN, (1 µg/L, n=3) or those DBPs with MRL≥2.5 µg/L (DIACM, DBCACM, BDCAA, DBCAA, and TBAA) (5 µg/L, n=4) and extracted following the analytical protocols described. To calculate analyte absolute recoveries and repeatability the peak areas obtained in fortified water samples and standard solutions at equivalent concentrations were compared. The lowest recoveries were found for HACMs, which affects the sensitivity of the method for these compounds. However, analyte losses during the extraction were automatically corrected in the quantification process because calibration solutions were prepared by fortifying LC-grade water at different concentrations and processing these solutions as if they were samples.

Table S3. Retention time and ions/SRM transitions monitored for GC-MS analysis of the target DBPs. The quantification ion/SRM transition is highlighted in bold.

Class	Analyte	SIM or SRM (m/z)	t_R	Linearity**		Recovery*
				Range(µg/L)	R^2	% (RSD)
THMs	DBCM	**129,**127,131	3.24	0.1-25	0.9979	108 (11)
	TBM	**173,**171,252	5.27	0.1-5	0.9978	124 (13)
	DCIM	**83,**127,175	3.73	0.1-10	0.9951	76 (19)
	BCIM	**127,**129,175	5.96	0.1-25	0.9959	79 (15)
	DBIM	**173**,171,127	8.10	0.1-5	0.9917	90 (19)
	CDIM	**175**,177,127	8.60	0.1-5	0.9959	70 (19)
	BDIM	**219**,127,140	10.38	0.25-5	0.9971	39 (15)
	TIM	**267,**394,127	12.30	0.1-5	0.9964	76 (17)
THALs	TCAL	**82,**84,111	2.77	0.25-2.5	0.9992	62 (10)
	BDCAL	83**,111**,128	4.81	0.25-2.5	0.9993	68 (23)
	DBCAL	127,**129**,157	7.49	0.25-2.5	0.9963	55 (21)
	TBAL	**173**,175,252	9.52	0.1-2.5	0.9935	70 (21)
HANs	CAN	**75,**77,48	3.74	0.25-10	0.9913	41 (21)
	BAN	**119**,121,79	6.34	0.1-2.5	0.9903	54 (15)
	IAN	**167,**127,139	9.28	0.1-2.5	0.9915	54 (24)
	DCAN	74,**82,**76	3.65	0.1-10	0.9971	96 (17)
	DBAN	118,**120**,199	8.60	0.1-2.5	0.9926	90 (27)
	BDCAN	108**,110,**154	4.02	1-10	0.9924	82 (17)
	DBCAN	**154,**152,79	7.06	0.25-5	0.9905	84 (10)
	TBAN	**198,**200,117	9.54	0.25-5	0.9921	78 (28)
HACMs	CACM	44,49,**93**	6.56	0.5-10	0.9941	12 (9)
	BACM	44,**137**,139	8.00	0.5-10	0.9965	17 (3)
	IACM	58,127,**185**	10.24	0.5-25	0.9934	23 (8)
	BCACM	44,**173**,93	9.50	0.25-10	0.9971	67 (8)
	DCACM	**44**,85,129	8.30	0.1-10	0.9919	60 (6)
	DBACM	44,217,**174**	10.76	0.1-10	0.9868	68 (9)
	CIACM	44,**219**,176	11.27	0.5-25	0.9911	32 (14)
	BIACM	138,220**,263**	12.38	0.25-10	0.9916	47 (8)
	DIACM	127,**184**,311	13.97	2.5-50	0.9921	23 (7)
	TCACM	**44,**82,98	10.01	0.05-5	0.9944	77 (7)
	BDCACM	**44**,126,82	11.34	0.1-10	0.9939	42 (13)
	DBCACM	**44**,207,251	12.57	2.5-10	0.9641	18 (5)
	TBACM	44,**172**,295	13.73	0.5-25	0.9923	39 (10)
HAAs	CAA	**77>49,** 79>51, 108>76	4.93	0.25-25	0.9910	59 (10)
	BAA	**121>93**, 123>95	6.07	0.25-25	0.9971	68 (9)
	IAA	**200>73**, 169>141	7.80	0.05-25	0.9971	73 (9)
	BCAA	**127>92**, 129>94	7.94	1-50	0.9952	89 (13)
	DCAA	**83>47**, 85>47, 111>83	6.11	0.5-25	0.9981	86 (9)
	DBAA	**171>92**, 173>94	10.13	0.1-25	0.9949	84 (11)
	CIAA	**234>79**, 175>48, 234>107	10.98	0.5-25	0.9952	60 (19)
	BIAA	**280>125**, 278>123, 221>94	12.47	0.1-2.5	0.9983	68 (21)
	DIAA	**326>171**, 326>199	14.14	0.05-2.5	0.9969	51 (25)
	TCAA	**117>82**, 119>84	7.46	0.1-25	0.9971	84 (17)
	BDCAA	**161>82,** 163>82	10.05	2.5-25	0.9913	65 (32)
	DBCAA	**187>159**, 209>128, 207>128	12.13	-	-	NR
	TBAA	**251>172,** 253>172	13.76	-	-	NR
	DCPA	**97>61**, 278<123, 187<105	6.44	0.05-5		68 (19)

*Average absolute recoveries observed at 0.5 µg/L (n=4) and relative standard deviation (RSD). In the case of regulated THMs, DBCM, and TBM, and the trihalo-HANs BDCAN, DBCAN, and TBAN, recoveries were investigated at 1 µg/L (n=3). For those analytes with MRL≥2.5 µg/L (DIACM, DBCACM, BDCAA, DBCAA, and TBAA, average absolute recoveries were studied at a concentration level of 5 µg/L (n=4). NR: Analyte not properly recovered (RSD>100 and absolute recovery <30).
**A minimum of 5 calibration points (exceptionally four) in the range 0.1-50 µg/L in the case of THMs, THALs, and HANs, and 0.05-50 µg/L in the case of HACMs, and HAAs were used to construct calibration curves.

VI. Targeted halogenated DBPs in water samples

Table S4. Concentrations of target halogenated DBPs in ng/L measured in disinfected water samples (n.d.= not detected).

Class	Analyte	DWTP1	DWTP2	DWTP3	DWTP4	MRL
THMs	DBCM	15	n.d.	n.d.	1.6	<0.10
	TBM	2.6	n.d.	n.d.	<0.1	<0.10
	DCIM	0.97	n.d.	n.d.	0.37	0.10
	BCIM	0.77	n.d.	n.d.	<0.1	0.10
	DBIM	0.19	n.d.	n.d.	n.d.	0.10
	CDIM	n.d.	n.d.	n.d.	n.d.	0.10
	BDIM	n.d.	n.d.	n.d.	n.d.	0.25
	TIM	n.d.	n.d.	n.d.	n.d.	0.10
THALs	TCAL	0.45	n.d.	n.d.	1.7	0.25
	BDCAL	0.41	n.d.	n.d.	0.30	0.25
	DBCAL	n.d.	n.d.	n.d.	n.d.	0.25
	TBAL	n.d.	n.d.	n.d.	n.d.	0.10
HANs	CAN	n.d.	n.d.	n.d.	n.d.	0.25
	BAN	n.d.	n.d.	n.d.	n.d.	0.10
	IAN	n.d.	n.d.	n.d.	n.d.	0.10
	DCAN	0.88	<0.1	n.d.	1.7	0.10
	DBAN	0.71	n.d.	n.d.	n.d.	0.10
	BDCAN	n.d.	n.d.	n.d.	n.d.	0.50
	DBCAN	n.d.	n.d.	n.d.	n.d.	0.25
	TBAN	n.d.	n.d.	n.d.	n.d.	0.25
HACMs	CACM	n.d.	n.d.	n.d.	n.d.	0.25
	BACM	n.d.	n.d.	n.d.	n.d.	0.50
	IACM	n.d.	n.d.	n.d.	n.d.	0.50
	BCACM	0.39	<0.1	n.d.	0.24	0.10
	DCACM	n.d.	<0.25	n.d.	1.1	0.25
	DBACM	n.d.	n.d.	n.d.	n.d.	0.10
	CIACM	n.d.	n.d.	n.d.	n.d.	0.50
	BIACM	n.d.	n.d.	n.d.	n.d.	0.25
	DIACM	n.d.	n.d.	n.d.	n.d.	2.5
	TCACM	n.d.	n.d.	n.d.	<0.05	0.05
	BDCACM	n.d.	n.d.	n.d.	n.d.	0.10
	DBCACM	n.d.	n.d.	n.d.	n.d.	2.5
	TBACM	n.d.	n.d.	n.d.	n.d.	0.50
HAAs	CAA	0.39	n.d.	n.d.	0.57	0.25
	BAA	0.38	n.d.	n.d.	<0.25	0.25
	IAA	<0.05	n.d.	0.05	<0.05	0.05
	BCAA	2.1	n.d.	n.d.	3.3	1.0
	DCAA	3.2	1.2	1.1	12	0.50
	DBAA	1.9	0.25	n.d.	0.49	0.10
	CIAA	0.61	n.d.	n.d.	0.62	0.05
	BIAA	0.12	n.d.	n.d.	n.d.	0.05
	DIAA	0.13	0.12	n.d.	n.d.	0.05
	TCAA	1.4	<0.1	0.30	11	0.10
	BDCAA	2.7	n.d.	n.d.	8.6	2.5
	DBCAA	n.d.	n.d.	n.d.	<10	10
	TBAA	n.d.	n.d.	n.d.	n.d.	10
	DPN	0.25	n.d.	n.d.	1.6	0.05

VII. Tranformation of DBP concentration of Cl-equivalent concentrations

To convert DBP concentrations into Cl-eq concentrations, the following formula was applied, in which the same atomic weight (35.45 Da) is assigned to all halogens present in the molecule (chlorine, bromine, and iodine) [1]:

$$\frac{\mu g\ of\ DBP\ as\ Cl-eq}{L} = \frac{DBP\ conc\ (\frac{\mu g}{L})}{DBP\ M.W.\ (\frac{g}{mol})} * (No.\ halogen\ atoms) * 35.45$$

Where *DBP conc* is the concentration of the DBP in µg/L and *DBP M.W.* is the molecular weight of the DBP (g/mol).

Reference

[1] M.J. Farré, K. Doederer, W. Gernjak, Y. Poussade, H. Weinberg, Disinfection by-products management in high quality recycled water, Water Supply, 12 (2012) 573-579.

VIII. Further interpretation of negative ESI-FT-ICR MS data

Search constraints: TIC>3,000,000; ≤800 Da, a mass error ± 0.2 ppm, and Nitrogen rule: TRUE, elemental composition: ^{12}C: 0–100, ^{1}H: 0–∞, ^{16}O: 0–80, ^{14}N: 0–3, ^{32}S: 0–2, ^{35}Cl: 0–5 and ^{79}Br: 0–3.
Formula filter: H/C≤2.5;O/C≤1;C,H and O>0, DBE≥0 and N and S≤1.

Table S5.Nitrogen-containing formulae in the investigated samples after search and formula filtration [a].

Sample code		No. of formulas in the 3 sample replicates	No. of verified formulas (in all replicates)	Theoretical mass (Da) $[M-H]^-$	Molecular formula [M]	DBE
DWTP1	IN	19	1	326.09725	$C_{12}H_{26}O_4BrN$	0
	OUT	24	0	-	-	-
DWTP2	IN	28	0	-	-	-
	OUT	28	3	288.02804	$C_{11}H_{12}O_6ClN$	6
				302.04369	$C_{12}H_{14}O_6ClN$	6
				314.04369	$C_{13}H_{14}O_6ClN$	7
DWTP3	IN	24	0	-	-	-
	OUT	22	0	-	-	-
DWTP4	IN	50	3	610.14959	$C_{30}H_{40}O_3Cl_2BrN$	10
				638.21727	$C_{33}H_{48}O_2Cl_2BrN$	9
				652.19654	$C_{33}H_{46}O_3Cl_2BrN$	10
	OUT	67	5	300.02804	$C_{12}H_{12}O_6Cl_1N$	7
				302.04369	$C_{12}H_{14}O_6Cl_1N$	6
				312.02804	$C_{13}H_{12}O_6Cl_1N$	8
				314.04369	*$C_{13}H_{14}O_6Cl_1N$*	*7*
				316.05934	$C_{13}H_{16}O_6Cl_1N$	6

[a] *Masses with equal intensity in IN and OUT are highlighted in italics and grey.*

Table S6.Sulfur-containing formulae in the investigated samples after search and formulae filtration [a].

Sample code		No. of formulas in the 3 sample replicates	No. of verified formulas (in all replicates)	Theoretical mass (Da) $[M-H]^-$	Molecular formula [M]	DBE
DWTP1	IN	30	5	413.0922	$C_{17}H_{32}O_2ClBrS$	1
				425.0922	$C_{18}H_{32}O_2ClBrS$	2
				427.10787	*$C_{18}H_{34}O_2ClBrS$*	*1*
				427.14425	*$C_{19}H_{38}OClBrS$*	*0*
				453.15990	*$C_{21}H_{40}OClBrS$*	*1*
	OUT	30	5	346.73820	$C_5H_3OBr_3S$	3
				427.10787	*$C_{18}H_{34}O_2ClBrS$*	*1*
				427.14425	*$C_{19}H_{38}OClBrS$*	*0*
				439.14425	$C_{20}H_{38}OClBrS$	1
				453.1599	*$C_{21}H_{40}OClBrS$*	*1*
DWTP2	IN	22	6	*411.11295*	*$C_{18}H_{34}OClBrS$*	*1*
				413.09222	*$C_{17}H_{32}O_2ClBrS$*	*1*
				413.12860	*$C_{18}H_{36}OClBrS$*	*0*
				425.09222	$C_{18}H_{32}O_2ClBrS$	2
				427.10787	$C_{18}H_{34}O_2ClBrS$	1
				427.14425	*$C_{18}H_{34}O_2ClBrS$*	*0*
	OUT	55	5	346.73820	$C_5H_3OBr_3S$	3
				411.11295	*$C_{18}H_{34}OClBrS$*	*1*
				413.09222	*$C_{17}H_{32}O_2ClBrS$*	*1*
				413.12860	*$C_{18}H_{36}OClBrS$*	*0*
				427.14425	*$C_{18}H_{34}O_2ClBrS$*	*0*
DWTP3	IN	23	5	425.09222	$C_{18}H_{32}O_2ClBrS$	2
				427.10787	*$C_{18}H_{34}O_2ClBrS$*	*1*
				427.14425	*$C_{18}H_{34}O_2ClBrS$*	*0*
				451.14425	*$C_{21}H_{40}OClBrS$*	*2*
				453.1599	*$C_{21}H_{40}OClBrS$*	*1*
	OUT	59	8	413.09222	$C_{17}H_{32}O_2ClBrS$	1
				427.10787	*$C_{18}H_{34}O_2ClBrS$*	*1*
				427.14425	*$C_{18}H_{34}O_2ClBrS$*	*0*
				439.14425	$C_{20}H_{38}OClBrS$	1
				451.14425	*$C_{21}H_{40}OClBrS$*	*2*
				453.1599	*$C_{21}H_{40}OClBrS$*	*1*
				477.00526	$C_{21}H_{15}O_9ClS$	14
				507.01582	$C_{22}H_{17}O_{10}ClS$	14
DWTP4	IN	18	5	*413.09222*	*$C_{17}H_{32}O_2ClBrS$*	*1*
				413.12860	*$C_{18}H_{36}OClBrS$*	*0*
				425.09222	*$C_{18}H_{32}O_2ClBrS$*	*2*
				427.10787	*$C_{18}H_{34}O_2ClBrS$*	*1*
				427.14425	*$C_{18}H_{34}O_2ClBrS$*	*0*
	OUT	24	4	*413.09222*	*$C_{17}H_{32}O_2ClBrS$*	*1*
				413.12860	*$C_{18}H_{36}OClBrS$*	*0*
				427.10787	*$C_{18}H_{34}O_2ClBrS$*	*1*
				427.14425	*$C_{18}H_{34}O_2ClBrS$*	*0*

[a] *Masses with equal intensity in IN and OUT are highlighted in italics and grey.*

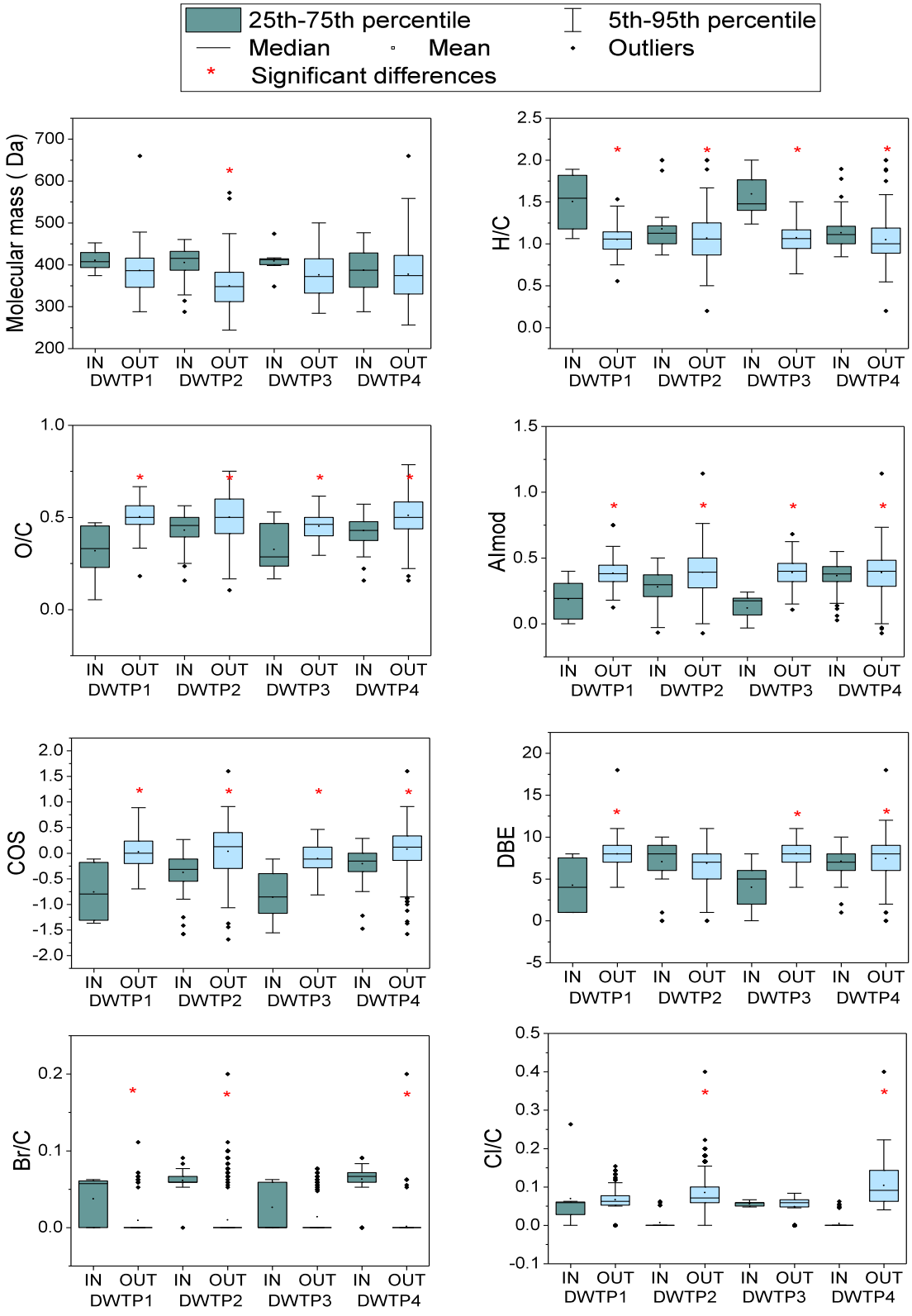


Figure S5. Box plots showing the properties of verified formulas in IN and OUT samples, after FT-ICR MS analysis.

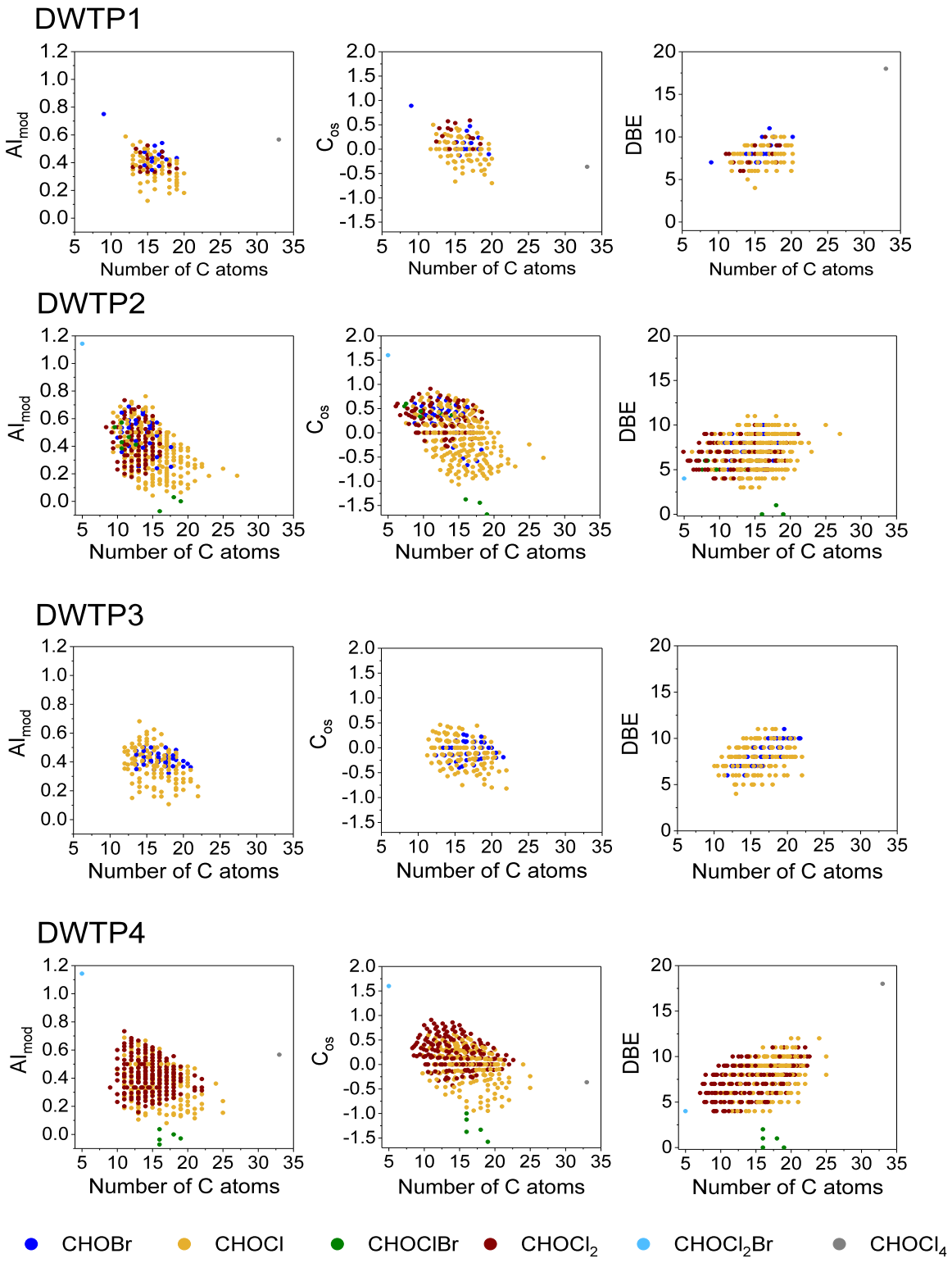


Figure S6. Plots showing DBE, AI_{mod}, and C*OS* versus the number of carbon for verified DBPs (*m/z* ions only present in disinfected water) according to negative ESI-FT-ICR MS analysis.

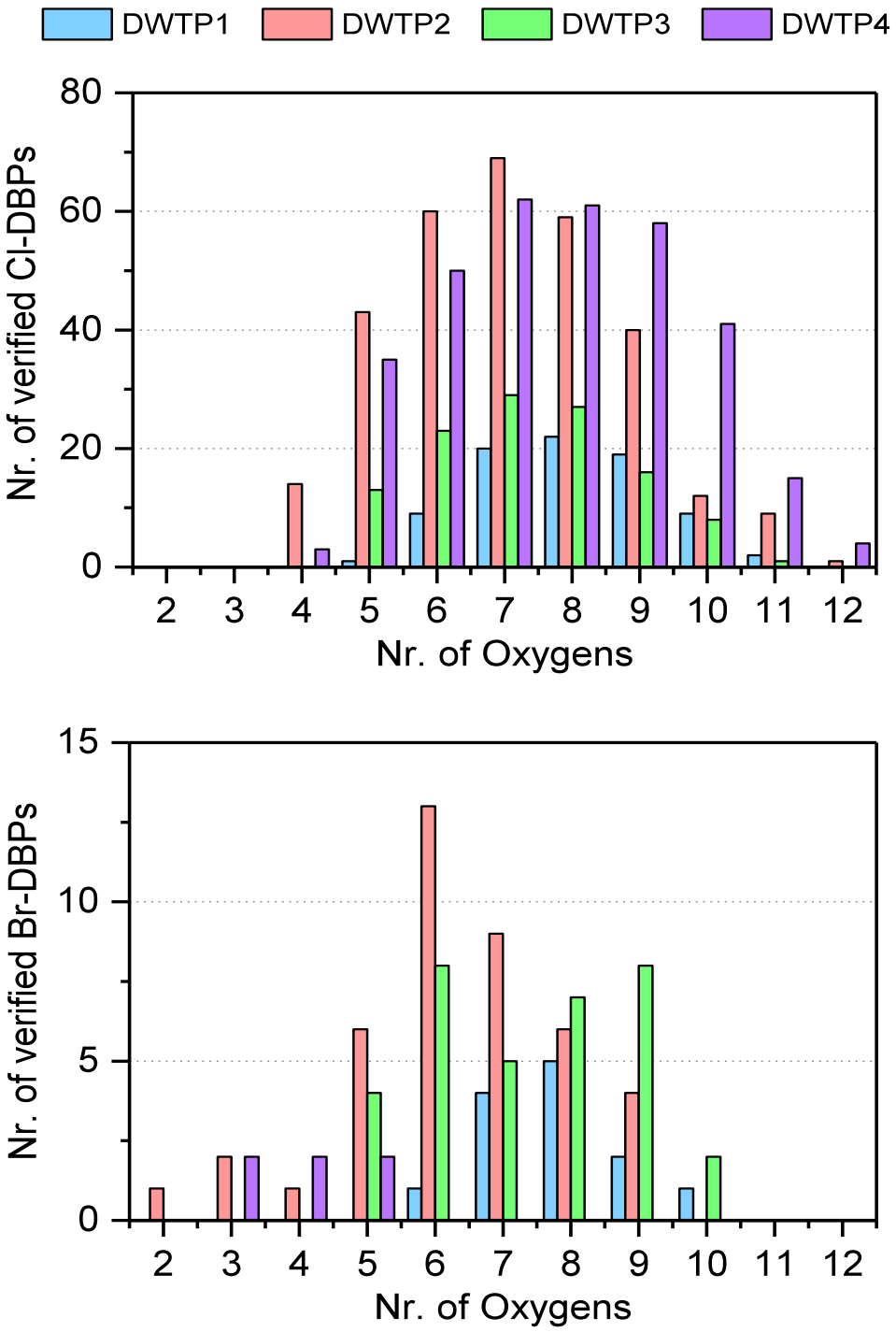


Figure S7. The number of verified chlorinated and brominated DBPs (CHO-type) in the investigated DBP mixtures against the number of oxygen atoms of each DBP composition according to negative ESI-FT-ICR MS analysis.

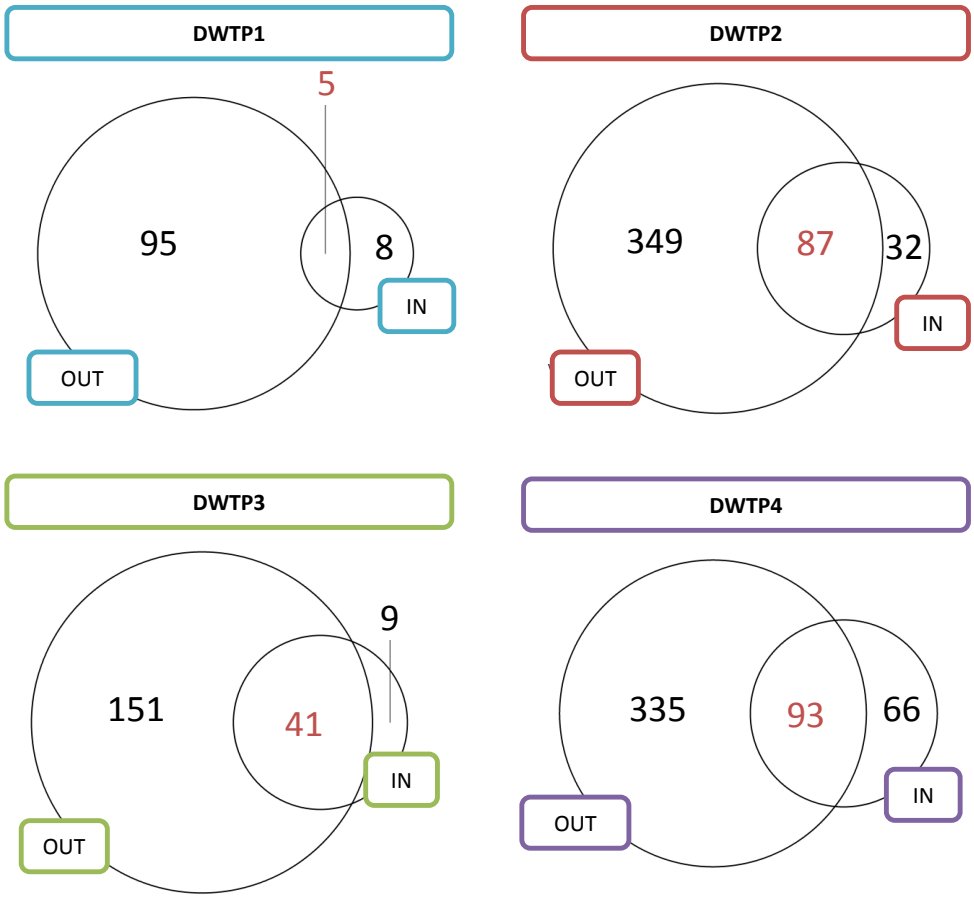


Figure S8. Venn diagrams showing the number of molecular formulae unique and common to non-disinfected (IN) and disinfected water (OUT) in each investigated drinking water treatment plant, after non-target FT-ICR MS analysis.

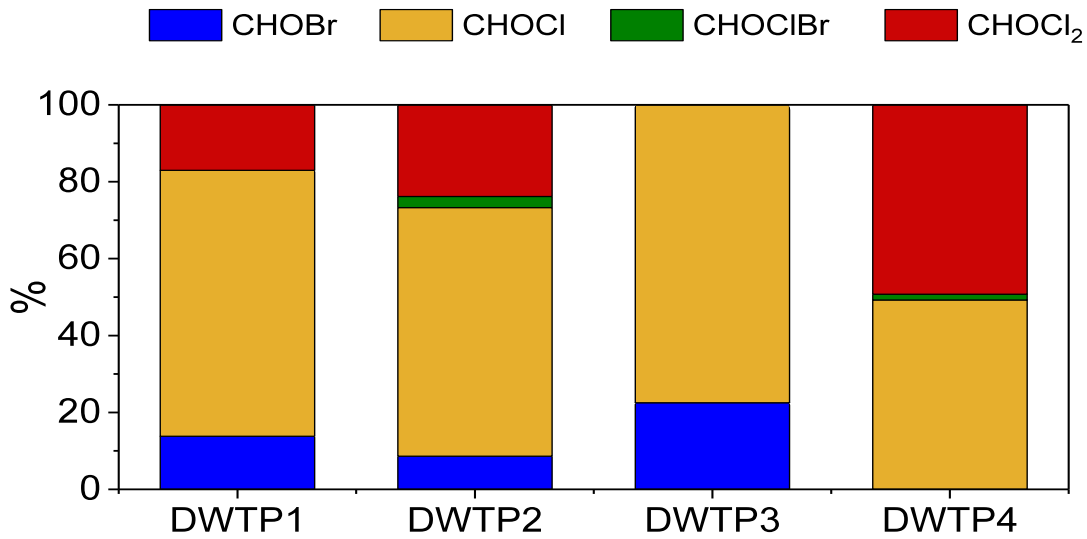


Figure S9. Contribution of each group of halogenated compounds to the chemodiversity of the investigated disinfected waters, after FT-ICR MS analysis. Y-axis shows the percent of verified molecular formulae.

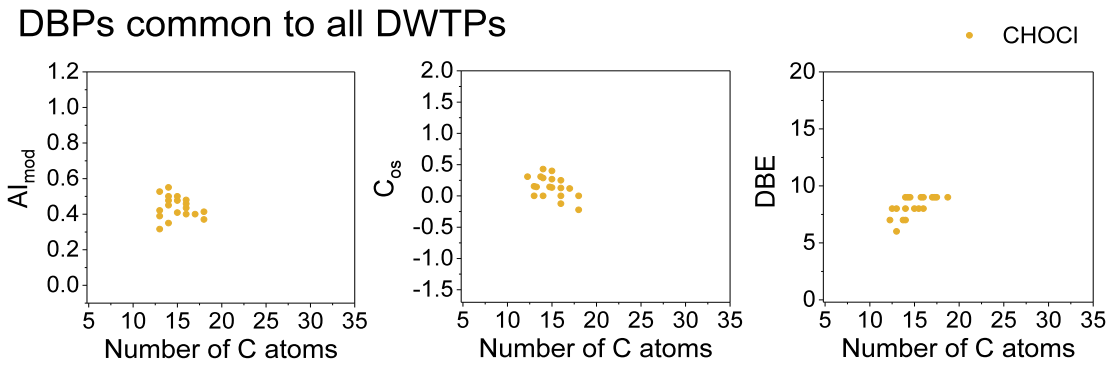


Figure S10. Plots showing DBE, AI_{mod}, and C_{OS} versus the number of carbon for verified DBPs (*m/z* ions only present in disinfected water) common to all DWTPs according to negative ESI-FT-ICR MS analysis.

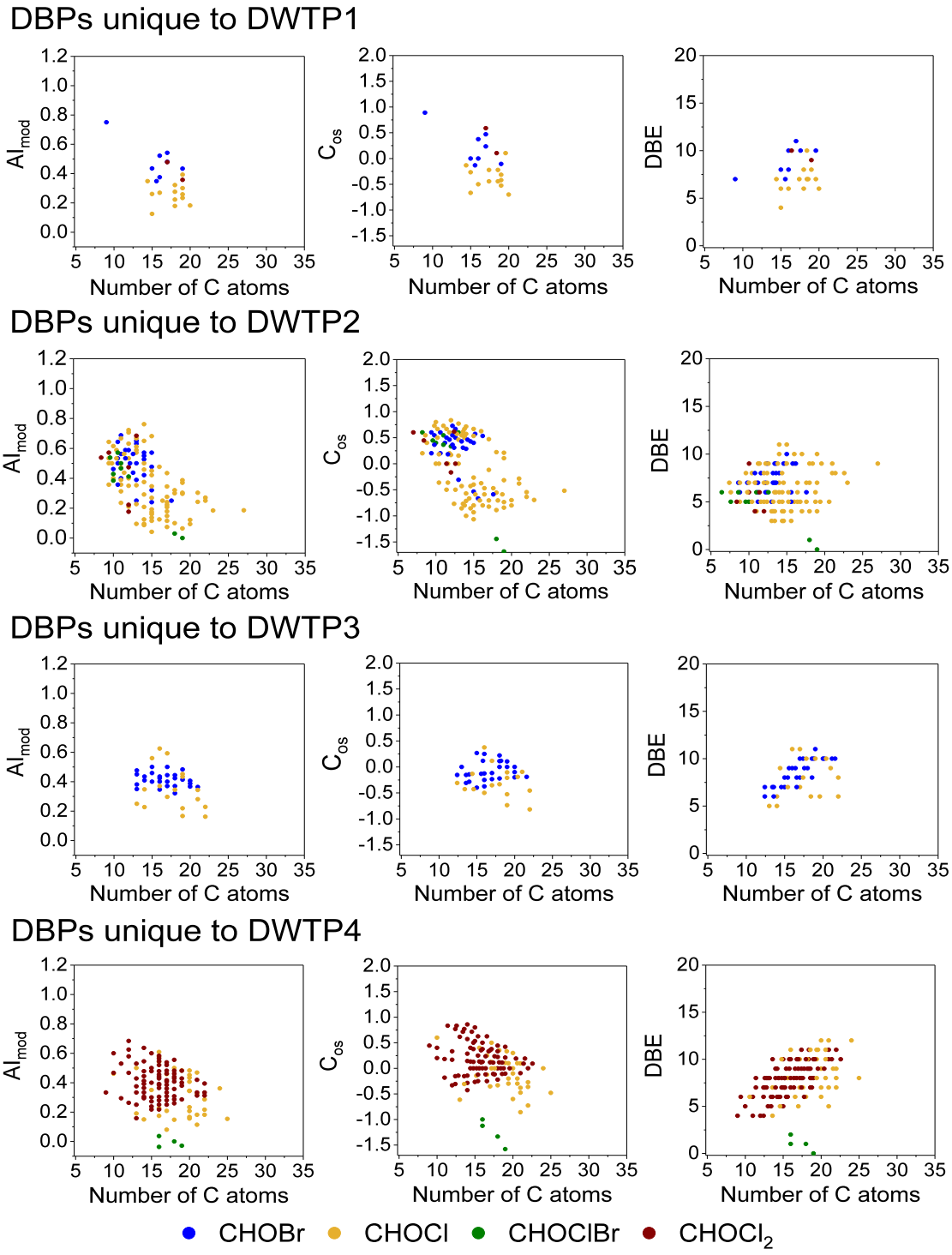


Figure S11. Plots showing DBE, AI_{mod}, and C_{OS} versus the number of carbon for unique verified DBPs (*m/z* ions only present in disinfected water) according to negative ESI-FT-ICR MS analysis.

Table S7. Statistics for comparison of the molecular mass of verified Cl and Br formulae in the investigated samples, after negative ESI-FT-ICR MS analysis**.**

		n	Mann-Whitney U* (2 independent groups: IN vs OUT)			Kruskal-Wallis** (various independent groups: DWTP_OUT samples)			
			Median	U	p-value	Median	$\chi^2_{(3)}$	p-value	Post-hoc Dunn's test (p<0.05)
DWTP1	IN	8	407	555	0.088		59.1	**<0.001**	*DWTP1 vs DWTP2* *DWTP3 vs DWTP2* *DWTP4 vs DWTP2*
	OUT	95	386			386			
DWTP2	IN	32	415	9533	**<0.001**				
	OUT	349	348			348			
DWTP3	IN	9	412	1017	**0.031**				
	OUT	151	372			372			
DWTP4	IN	66	387	14530	0.142				
	OUT	335	374			374			

*When p-value <0.05, the molecular mass of the Cl and Br-formulae before and after disinfection are significantly different with a significance level of 5%. Overlapping features between IN and OUT were removed.

**When p-value <0.05, the molecular mass of the Cl and Br-formulae in disinfected water of the different DWTPs are significantly different with a significance level of 5%. Pairwise comparison with a posthoc Dunn's test allows identification of the differences.

Table S8. Statistics for comparison of the H/C content of verified Cl and Br formulae in the investigated samples, after negative ESI-FT-ICR MS analysis**.**

		n	Mann-Whitney U* (2 independent groups: IN vs OUT)			Kruskal-Wallis** (various independent groups: DWTP_OUT samples)			
			Median	U	p-value	Median	$\chi^2_{(3)}$	p-value	Post-hoc Dunn's test (p<0.05)
DWTP1	IN	8	1.55	706	**<0.001**		2.81	0.422	-
	OUT	95	1.06			1.06			
DWTP2	IN	32	1.13	7262	0.054				
	OUT	349	1.06			1.06			
DWTP3	IN	9	1.48	1348	**<0.001**				
	OUT	151	1.06			1.06			
DWTP4	IN	66	1.11	16001	**0.001**				
	OUT	335	1.00			1.00			

*When p-value <0.05, the H/C content of verified Cl and Br-formulae before and after disinfection are significantly different with a significance level of 5%. Overlapping features between IN and OUT were removed.

**When p-value <0.05, the H/C content of verified DBPs in disinfected water of the different DWTPs are significantly different with a significance level of 5%. Pairwise comparison with a posthoc Dunn's test allows identification of the differences.

Table S9. Statistics for comparison of the O/C content of verified Cl and Br formulae in the investigated samples, after negative ESI-FT-ICR MS analysis**.**

		n	Mann-Whitney U* (2 independent groups: IN vs OUT)			Kruskal-Wallis** (various independent groups: DWTP_OUT samples)			
			Median	U	p-value	Median	$\chi^2_{(3)}$	p-value	Post-hoc Dunn's test (p<0.05)
DWTP1	IN	8	0.33	128	**<0.001**		38.9	**<0.001**	*DWTP4 vs DWTP3*
	OUT	95	0.50			0.50			*DWTP1 vs DWTP3*
DWTP2	IN	32	0.46	4175	**0.001**				*DWTP2 vs DWTP3*
	OUT	349	0.50			0.50			
DWTP3	IN	9	0.29	362	**0.007**				
	OUT	151	0.46			0.46			
DWTP4	IN	66	0.43	8145	**<0.001**				
	OUT	335	0.50			0.50			

*When p-value <0.05, the O/C content of verified Cl and Br-formulae before and after disinfection are significantly different with a significance level of 5%. Overlapping features between IN and OUT were removed.

**When p-value <0.05, the O/C content of verified DBPs in disinfected water of the different DWTPs are significantly different with a significance level of 5%. Pairwise comparison with a posthoc Dunn's test allows identification of the differences.

Table S10. Statistics for comparison of the AImod of verified Cl and Br formulae in the investigated samples, after negative ESI-FT-ICR MS analysis**.**

		n	Mann-Whitney U* (2 independent groups: IN vs OUT)			Kruskal-Wallis** (various independent groups: DWTP_OUT samples)			
			Median	U	p-value	Median	$\chi^2_{(3)}$	p-value	Post-hoc Dunn's test (p<0.05)
DWTP1	IN	8	0.19	139	**<0.001**		0.38	0.945	-
	OUT	95	0.38			0.38			
DWTP2	IN	32	0.36	5213	0.132				
	OUT	349	0.39			0.39			
DWTP3	IN	9	0.17	93	**<0.001**				
	OUT	151	0.40			0.40			
DWTP4	IN	66	0.38	12270	0.247				
	OUT	335	0.40			0.4			

*When p-value <0.05, the AImod content of verified Cl and Br-formulae before and after disinfection are significantly different with a significance level of 5%. Overlapping features between IN and OUT were removed.

**When p-value <0.05, the AImod content of verified DBPs in disinfected water of the different DWTPs are significantly different with a significance level of 5%. Pairwise comparison with a posthoc Dunn's test allows identification of the differences.

Table S 11. Statistics for comparison of the C_{OS} of verified Cl and Br formulae in the investigated samples, after negative ESI-FT-ICR MS analysis**.**

		n	Mann-Whitney U* (2 independent groups: IN vs OUT)			Kruskal-Wallis** (various independent groups: DWTP_OUT samples)			
			Median	U	p-value	Median	$\chi^2_{(3)}$	p-value	Post-hoc Dunn's test (p<0.05)
DWTP1	IN	8	-0.80	115	**<0.001**		34.2	**<0.001**	*DWTP4 vs DWTP3*
	OUT	95	0			0			*DWTP1 vs DWTP3*
DWTP2	IN	32	-0.13	4129	**<0.001**				*DWTP2 vs DWTP3*
	OUT	349	0.13			0.13			
DWTP3	IN	9	-0.86	184	**<0.001**				
	OUT	151	-0.12			-0.12			
DWTP4	IN	66	-0.15	8015	**<0.001**				
	OUT	335	0.12			0.12			

*When p-value <0.05, the **C_{OS}** content of verified Cl and Br-formulae before and after disinfection are significantly different with a significance level of 5%. Overlapping features between IN and OUT were removed.

When p-value <0.05, the **C_{OS} content of verified DBPs in disinfected water of the different DWTPs are significantly different with a significance level of 5%. Pairwise comparison with a posthoc Dunn's test allows identification of the differences.

Table S12. Statistics for comparison of the DBE of verified Cl and Br formulae in the investigated samples, after negative ESI-FT-ICR MS analysis**.**

		n	Mann-Whitney U* (2 independent groups: IN vs OUT)			Kruskal-Wallis** (various independent groups: DWTP_OUT samples)			
			Median	U	p-value	Median	$\chi^2_{(3)}$	p-value	Post-hoc Dunn's test (p<0.05)
DWTP1	IN	8	4	168	**0.002**		49.7	**<0.001**	*DWTP3 vs DWTP2*
	OUT	95	8			8			*DWTP3 vs DWTP4*
DWTP2	IN	32	8	7013	0.126				*DWTP1 vs DWTP2*
	OUT	349	7			7			*DWTP4 vs DWTP2*
DWTP3	IN	9	5	196	**<0.001**				
	OUT	151	8			8			
DWTP4	IN	66	7	12294	0.253				
	OUT	335	8			8			

*When p-value <0.05, the DBE content of verified Cl and Br-formulae before and after disinfection are significantly different with a significance level of 5%. Overlapping features between IN and OUT were removed.

**When p-value <0.05, the DBE content of verified DBPs in disinfected water of the different DWTPs are significantly different with a significance level of 5%. Pairwise comparison with a posthoc Dunn's test allows identification of the differences.

Table S13. List of verified formulae of the 19 DBPs common to all four disinfected water samples according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

Common to all DWTPs	
Molecular formula	***Theoretical mass of the negative ion***
C14 H13 O6 Cl1	311.03279
C13 H11 O7 Cl1	313.01206
C13 H13 O7 Cl1	315.02771
C13 H15 O7 Cl1	317.04336
C14 H13 O7 Cl1	327.02771
C13 H13 O8 Cl1	331.02262
C14 H11 O8 Cl1	341.00697
C14 H13 O8 Cl1	343.02262
C14 H15 O8 Cl1	345.03827
C16 H15 O7 Cl1	353.04336
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C15 H15 O8 Cl1	357.03827
C16 H15 O8 Cl1	369.03827
C15 H13 O9 Cl1	371.01754
C18 H19 O7 Cl1	381.07466
C17 H17 O8 Cl1	383.05392
C16 H15 O9 Cl1	385.03319
C17 H17 O9 Cl1	399.04884
C18 H19 O9 Cl1	413.06449

Table S14. List of verified formulae of the 23 DBPs unique to DWTP1 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP1-unique	
Molecular formula	***Theoretical mass of the negative ion***
C9 H5 O6 Br1	286.91968
C15 H23 O6 Cl1	333.11104
C15 H17 O7 Cl1	343.05901
C16 H21 O6 Cl1	343.09539
C15 H19 O7 Cl1	345.07466
C15 H15 O7 Br1	384.99284
C18 H23 O7 Cl1	385.10596
C15 H17 O7 Br1	387.00849
C18 H21 O8 Cl1	399.08522
C19 H25 O7 Cl1	399.12161
C18 H25 O8 Cl1	403.11652
C19 H23 O8 Cl1	413.10087
C16 H17 O8 Br1	415.00341
C19 H25 O8 Cl1	415.11652
C20 H29 O7 Cl1	415.15291
C18 H23 O9 Cl1	417.09579
C16 H13 O9 Br1	426.96702
C17 H15 O9 Br1	440.98267
C19 H19 O10 Cl1	441.05940
C19 H19 O8 Br1	453.01906
C17 H13 O10 Br1	454.96194
C17 H14 O11 Cl2	462.98405
C19 H20 O10 Cl2	477.03608

Table S15. List of verified formulae of the 124 DBPs unique to DWTP2 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP2-unique	
Molecular formula	***Theoretical mass of the negative ion***
C10 H9 O5 Cl1	243.00658
C11 H13 O4 Cl1	243.04296
C10 H11 O5 Cl1	245.02223
C11 H9 O5 Cl1	255.00658
C10 H7 O6 Cl1	256.98584
C11 H11 O5 Cl1	257.02223
C12 H15 O4 Cl1	257.05861
C10 H9 O6 Cl1	259.00149
C10 H11 O6 Cl1	261.01714
C11 H15 O5 Cl1	261.05353
C9 H8 O5 Cl2	264.96761
C12 H9 O5 Cl1	267.00658
C10 H7 O7 Cl1	272.98076
C13 H19 O4 Cl1	273.08991
C11 H13 O6 Cl1	275.03279
C12 H17 O5 Cl1	275.06918
C13 H9 O5 Cl1	279.00658
C12 H7 O6 Cl1	280.98584
C13 H11 O5 Cl1	281.02223
C14 H15 O4 Cl1	281.05861
C14 H17 O4 Cl1	283.07426
C11 H7 O7 Cl1	284.98076
C14 H19 O4 Cl1	285.08991
C10 H9 O5 Br1	286.95606
C11 H9 O7 Cl1	286.99641
C14 H21 O4 Cl1	287.10556
C14 H23 O4 Cl1	289.12121
C13 H21 O5 Cl1	291.10048
C10 H8 O6 Cl2	292.96252
C12 H7 O7 Cl1	296.98076
C15 H19 O4 Cl1	297.08991
C11 H9 O5 Br1	298.95606
C15 H21 O4 Cl1	299.10556
C10 H7 O6 Br1	300.93533
C15 H23 O4 Cl1	301.12121
C10 H9 O6 Br1	302.95098
C11 H9 O8 Cl1	302.99132
C15 H25 O4 Cl1	303.13686
C10 H11 O6 Br1	304.96663

DWTP2-unique (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C12 H12 O5 Cl2	304.99891
C11 H11 O8 Cl1	305.00697
C14 H23 O5 Cl1	305.11613
C9 H8 O5 Cl1 Br1	308.91709
C11 H7 O6 Br1	312.93533
C11 H9 O6 Br1	314.95098
C12 H9 O8 Cl1	314.99132
C12 H11 O8 Cl1	317.00697
C15 H23 O5 Cl1	317.11613
C10 H9 O7 Br1	318.94589
C14 H7 O7 Cl1	320.98076
C12 H16 O6 Cl2	325.02512
C13 H9 O8 Cl1	326.99132
C11 H9 O7 Br1	330.94589
C12 H9 O9 Cl1	330.98624
C11 H11 O7 Br1	332.96154
C12 H11 O9 Cl1	333.00189
C14 H21 O7 Cl1	335.09031
C15 H25 O6 Cl1	335.12669
C10 H8 O6 Cl1 Br1	336.91201
C10 H10 O6 Cl1 Br1	338.92766
C13 H9 O6 Br1	338.95098
C14 H9 O8 Cl1	338.99132
C17 H21 O5 Cl1	339.10048
C12 H16 O7 Cl2	341.02004
C17 H23 O5 Cl1	341.11613
C12 H9 O7 Br1	342.94589
C13 H9 O9 Cl1	342.98624
C17 H25 O5 Cl1	343.13178
C13 H8 O7 Cl2	344.95744
C11 H9 O8 Br1	346.94081
C13 H17 O6 Br1	347.01358
C13 H13 O9 Cl1	347.01754
C15 H21 O7 Cl1	347.09031
C11 H10 O6 Cl1 Br1	350.92766
C15 H9 O8 Cl1	350.99132
C10 H10 O7 Cl1 Br1	354.92257
C13 H9 O7 Br1	354.94589
C15 H19 O5 Br1	357.03431

Table S17. (cont.)

DWTP2-unique (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C17 H23 O6 Cl1	357.11104
C12 H9 O8 Br1	358.94081
C15 H21 O5 Br1	359.04996
C17 H25 O6 Cl1	359.12669
C12 H11 O8 Br1	360.95646
C15 H21 O8 Cl1	363.08522
C11 H10 O7 Cl1 Br1	366.92257
C19 H25 O5 Cl1	367.13178
C14 H11 O7 Br1	368.96154
C18 H23 O6 Cl1	369.11104
C13 H11 O8 Br1	372.95646
C14 H11 O10 Cl1	372.9968
C17 H23 O7 Cl1	373.10596
C13 H13 O8 Br1	374.97211
C17 H25 O7 Cl1	375.12161
C18 H29 O6 Cl1	375.15799
C16 H23 O8 Cl1	377.10087
C17 H27 O7 Cl1	377.13726
C12 H12 O7 Cl1 Br1	380.93822
C14 H11 O8 Br1	384.95646
C15 H13 O10 Cl1	387.01245
C17 H25 O8 Cl1	391.11652
C19 H21 O7 Cl1	395.09031
C14 H11 O9 Br1	400.95137
C17 H23 O6 Br1	401.06053
C14 H13 O9 Br1	402.96702
C15 H13 O11 Cl1	403.00737
C17 H21 O9 Cl1	403.08014
C19 H31 O7 Cl1	405.16856
C18 H34 O3 Cl1 Br1	411.13071
C19 H38 O2 Cl1 Br1	411.1671
C15 H11 O9 Br1	412.95137
C15 H13 O9 Br1	414.96702
C16 H13 O11 Cl1	415.00737
C20 H31 O7 Cl1	417.16856
C17 H15 O11 Cl1	429.02302
C20 H31 O8 Cl1	433.16347
C22 H29 O7 Cl1	439.15291

DWTP2-unique (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C18 H19 O11 Cl1	445.05432
C21 H25 O9 Cl1	455.11144
C22 H29 O8 Cl1	455.14782
C19 H19 O11 Cl1	457.05432
C21 H27 O9 Cl1	457.12709
C19 H21 O11 Cl1	459.06997
C23 H33 O8 Cl1	471.17912
C27 H37 O11 Cl1	571.19517

Table S16. List of verified formulae of the 44 DBPs unique to DWTP3 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP3-unique	
Molecular formula	***Theoretical mass of the negative ion***
C14 H17 O5 Cl1	299.06918
C13 H17 O6 Cl1	303.06409
C15 H13 O5 Cl1	307.03788
C14 H19 O6 Cl1	317.07974
C16 H19 O5 Cl1	325.08483
C13 H13 O5 Br1	326.98736
C13 H15 O5 Br1	329.00301
C14 H15 O5 Br1	341.00301
C13 H13 O6 Br1	342.98228
C13 H15 O6 Br1	344.99793
C15 H17 O5 Br1	355.01866
C14 H15 O6 Br1	356.99793
C17 H13 O7 Cl1	363.02771
C16 H11 O8 Cl1	365.00697
C15 H15 O6 Br1	368.99793
C17 H21 O7 Cl1	371.09031
C16 H17 O6 Br1	383.01358
C18 H21 O7 Cl1	383.09031
C16 H19 O6 Br1	385.02923
C19 H27 O6 Cl1	385.14234
C19 H19 O7 Cl1	393.07466
C15 H13 O8 Br1	398.97211
C16 H17 O7 Br1	399.00849
C19 H19 O8 Cl1	409.06957
C17 H17 O7 Br1	411.00849
C17 H19 O7 Br1	413.02414
C19 H27 O8 Cl1	417.13217
C17 H15 O8 Br1	424.98776
C16 H15 O9 Br1	428.98267
C17 H17 O9 Br1	442.99832
C18 H21 O8 Br1	443.03471
C22 H33 O7 Cl1	443.18421
C18 H17 O9 Br1	454.99832
C18 H19 O9 Br1	457.01397
C19 H17 O9 Br1	466.99832
C20 H21 O8 Br1	467.03471
C19 H19 O9 Br1	469.01397
C21 H23 O10 Cl1	469.0907

DWTP3-unique (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C18 H17 O10 Br1	470.99324
C21 H25 O10 Cl1	471.10635
C22 H29 O9 Cl1	471.14274
C20 H21 O9 Br1	483.02962
C21 H23 O9 Br1	497.04527
C20 H21 O10 Br1	499.02454

Table S17. List of verified formulae of the 121 DBPs unique to DWTP4 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP4-unique	
Molecular formula	***Theoretical mass of the negative ion***
C13 H13 O4 Cl1	267.04296
C10 H9 O7 Cl1	274.99641
C10 H8 O5 Cl2	276.96761
C10 H10 O5 Cl2	278.98326
C9 H10 O6 Cl2	282.97817
C13 H19 O5 Cl1	289.08483
C11 H10 O5 Cl2	290.98326
C11 H14 O5 Cl2	295.01456
C12 H8 O5 Cl2	300.96761
C12 H10 O5 Cl2	302.98326
C12 H16 O5 Cl2	309.03021
C13 H14 O5 Cl2	319.01456
C13 H16 O5 Cl2	321.03021
C14 H14 O5 Cl2	331.01456
C14 H16 O5 Cl2	333.03021
C16 H13 O6 Cl1	335.03279
C14 H18 O5 Cl2	335.04586
C14 H10 O6 Cl2	342.97817
C14 H12 O6 Cl2	344.99382
C12 H8 O8 Cl2	348.95235
C14 H16 O6 Cl2	349.02512
C14 H19 O8 Cl1	349.06957
C13 H18 O7 Cl2	355.03569
C15 H14 O6 Cl2	359.00947
C12 H10 O9 Cl2	366.96292
C16 H13 O8 Cl1	367.02262
C15 H14 O7 Cl2	375.00439
C16 H18 O6 Cl2	375.04077
C13 H10 O9 Cl2	378.96292
C16 H11 O9 Cl1	381.00189
C15 H20 O7 Cl2	381.05134
C16 H14 O7 Cl2	387.00439
C16 H16 O7 Cl2	389.02004
C15 H15 O10 Cl1	389.02810
C16 H21 O9 Cl1	391.08014
C16 H20 O7 Cl2	393.05134
C15 H18 O8 Cl2	395.03060
C13 H12 O10 Cl2	396.97348
C13 H14 O10 Cl2	398.98913

DWTP4-unique (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C16 H12 O8 Cl2	400.98365
C17 H16 O7 Cl2	401.02004
C17 H18 O7 Cl2	403.03569
C16 H19 O10 Cl1	405.05940
C17 H25 O9 Cl1	407.11144
C14 H12 O10 Cl2	408.97348
C16 H20 O8 Cl2	409.04625
C14 H14 O10 Cl2	410.98913
C15 H18 O9 Cl2	411.02552
C17 H15 O10 Cl1	413.02810
C16 H28 O5 Cl1 Br1	413.07359
C17 H14 O8 Cl2	414.99930
C16 H30 O5 Cl1 Br1	415.08924
C16 H12 O9 Cl2	416.97857
C17 H16 O8 Cl2	417.01495
C15 H10 O10 Cl2	418.95783
C16 H14 O9 Cl2	418.99422
C17 H18 O8 Cl2	419.03060
C17 H21 O10 Cl1	419.07505
C18 H25 O9 Cl1	419.11144
C16 H16 O9 Cl2	421.00987
C17 H20 O8 Cl2	421.04625
C15 H14 O10 Cl2	422.98913
C16 H18 O9 Cl2	423.02552
C19 H17 O9 Cl1	423.04884
C20 H21 O8 Cl1	423.08522
C14 H12 O11 Cl2	424.96840
C15 H16 O10 Cl2	425.00478
C18 H15 O10 Cl1	425.02810
C16 H20 O9 Cl2	425.04117
C20 H23 O8 Cl1	425.10087
C14 H14 O11 Cl2	426.98405
C18 H34 O4 Cl1 Br1	427.12563
C19 H38 O3 Cl1 Br1	427.16201
C17 H14 O9 Cl2	430.99422
C18 H18 O8 Cl2	431.03060
C20 H29 O8 Cl1	431.14782
C21 H33 O7 Cl1	431.18421
C16 H12 O10 Cl2	432.97348

Table S19. (cont).

DWTP4-unique (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C18 H20 O8 Cl2	433.04625
C16 H14 O10 Cl2	434.98913
C17 H18 O9 Cl2	435.02552
C18 H22 O8 Cl2	435.06190
C16 H16 O10 Cl2	437.00478
C17 H20 O9 Cl2	437.04117
C20 H19 O9 Cl1	437.06449
C21 H25 O8 Cl1	439.11652
C22 H31 O7 Cl1	441.16856
C18 H14 O9 Cl2	442.99422
C18 H16 O9 Cl2	445.00987
C19 H20 O8 Cl2	445.04625
C18 H18 O9 Cl2	447.02552
C17 H16 O10 Cl2	449.00478
C16 H14 O11 Cl2	450.98405
C17 H18 O10 Cl2	451.02043
C18 H22 O9 Cl2	451.05682
C17 H20 O10 Cl2	453.03608
C20 H19 O10 Cl1	453.05940
C20 H25 O10 Cl1	459.10635
C21 H29 O9 Cl1	459.14274
C18 H16 O10 Cl2	461.00478
C19 H20 O9 Cl2	461.04117
C20 H27 O10 Cl1	461.12200
C18 H20 O10 Cl2	465.03608
C21 H19 O10 Cl1	465.05940
C20 H17 O11 Cl1	467.03867
C22 H27 O9 Cl1	469.12709
C20 H21 O11 Cl1	471.06997
C19 H18 O10 Cl2	475.02043
C20 H25 O11 Cl1	475.10127
C18 H16 O11 Cl2	476.99970
C19 H22 O10 Cl2	479.05173
C19 H16 O11 Cl2	488.99970
C22 H29 O11 Cl1	503.13257
C21 H24 O10 Cl2	505.06738
C21 H20 O11 Cl2	517.03100
C18 H20 O8 Cl2	476.99970

DWTP4-unique (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C22 H22 O11 Cl2	531.04665
C22 H24 O11 Cl2	533.06230
C21 H22 O12 Cl2	535.04156
C24 H25 O12 Cl1	539.09618
C25 H35 O11 Cl1	545.17952
C22 H24 O12 Cl2	549.05721

Table S18. List of verified formulae of the 49 DBPs common to DWTP1 and DWTP2 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP1+DWTP2	
Molecular formula	***Theoretical mass of the negative ion***
C12 H9 O7 Cl1	298.99641
C13 H13 O6 Cl1	299.03279
C13 H15 O6 Cl1	301.04844
C14 H13 O6 Cl1	311.03279
C15 H17 O5 Cl1	311.06918
C13 H11 O7 Cl1	313.01206
C13 H13 O7 Cl1	315.02771
C13 H15 O7 Cl1	317.04336
C14 H13 O7 Cl1	327.02771
C13 H13 O8 Cl1	331.02262
C16 H17 O6 Cl1	339.06409
C14 H11 O8 Cl1	341.00697
C14 H13 O8 Cl1	343.02262
C14 H15 O8 Cl1	345.03827
C14 H17 O8 Cl1	347.05392
C13 H14 O7 Cl2	351.00439
C16 H15 O7 Cl1	353.04336
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C15 H15 O8 Cl1	357.03827
C15 H17 O8 Cl1	359.05392
C14 H16 O7 Cl2	365.02004
C16 H15 O8 Cl1	369.03827
C17 H19 O7 Cl1	369.07466
C15 H13 O9 Cl1	371.01754
C15 H15 O9 Cl1	373.03319
C16 H19 O8 Cl1	373.06957
C16 H21 O8 Cl1	375.08522
C14 H12 O8 Cl2	376.98365
C18 H19 O7 Cl1	381.07466
C17 H17 O8 Cl1	383.05392
C16 H15 O9 Cl1	385.03319
C17 H19 O8 Cl1	385.06957
C16 H17 O9 Cl1	387.04884
C15 H14 O8 Cl2	390.99930
C14 H12 O9 Cl2	392.97857
C15 H16 O8 Cl2	393.01495
C14 H14 O9 Cl2	394.99422

DWTP1+DWTP2 (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C17 H17 O9 Cl1	399.04884
C16 H15 O10 Cl1	401.02810
C17 H19 O9 Cl1	401.06449
C16 H17 O10 Cl1	403.04375
C15 H12 O9 Cl2	404.97857
C16 H18 O8 Cl2	407.03060
C18 H19 O9 Cl1	413.06449
C17 H17 O10 Cl1	415.04375
C19 H19 O9 Cl1	425.06449
C20 H23 O9 Cl1	441.09579
C19 H21 O10 Cl1	443.07505

Table S19. List of verified formulae of the 48 DBPs common to DWTP1 and DWTP3 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP1+DWTP3	
Molecular formula	***Theoretical mass of the negative ion***
C13 H13 O6 Cl1	299.03279
C13 H15 O6 Cl1	301.04844
C14 H13 O6 Cl1	311.03279
C15 H17 O5 Cl1	311.06918
C13 H11 O7 Cl1	313.01206
C14 H15 O6 Cl1	313.04844
C13 H13 O7 Cl1	315.02771
C13 H15 O7 Cl1	317.04336
C14 H13 O7 Cl1	327.02771
C14 H15 O7 Cl1	329.04336
C13 H13 O8 Cl1	331.02262
C14 H19 O7 Cl1	333.07466
C16 H17 O6 Cl1	339.06409
C14 H11 O8 Cl1	341.00697
C15 H15 O7 Cl1	341.04336
C14 H13 O8 Cl1	343.02262
C14 H15 O8 Cl1	345.03827
C16 H15 O7 Cl1	353.04336
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C15 H15 O8 Cl1	357.03827
C16 H19 O7 Cl1	357.07466
C15 H17 O8 Cl1	359.05392
C16 H15 O8 Cl1	369.03827
C17 H19 O7 Cl1	369.07466
C14 H13 O7 Br1	370.97719
C15 H13 O9 Cl1	371.01754
C16 H17 O8 Cl1	371.05392
C14 H15 O7 Br1	372.99284
C16 H19 O8 Cl1	373.06957
C16 H21 O8 Cl1	375.08522
C18 H19 O7 Cl1	381.07466
C17 H17 O8 Cl1	383.05392
C16 H15 O9 Cl1	385.03319
C17 H19 O8 Cl1	385.06957
C16 H17 O9 Cl1	387.04884
C17 H17 O9 Cl1	399.04884

DWTP1+DWTP3 (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C15 H15 O8 Br1	400.98776
C17 H19 O9 Cl1	401.06449
C16 H15 O8 Br1	412.98776
C18 H19 O9 Cl1	413.06449
C17 H17 O8 Br1	427.00341
C18 H17 O10 Cl1	427.04375
C19 H23 O9 Cl1	429.09579
C19 H25 O9 Cl1	431.11144
C20 H23 O9 Cl1	441.09579
C19 H21 O10 Cl1	443.07505
C19 H23 O10 Cl1	445.09070

Table S20. List of verified formulae of the 47 DBPs common to DWTP1 and DWTP4 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP1+DWTP4	
Molecular formula	***Theoretical mass of the negative ion***
C12 H9 O7 Cl1	298.99641
C14 H13 O6 Cl1	311.03279
C13 H11 O7 Cl1	313.01206
C13 H13 O7 Cl1	315.02771
C13 H15 O7 Cl1	317.04336
C14 H13 O7 Cl1	327.02771
C13 H13 O8 Cl1	331.02262
C14 H11 O8 Cl1	341.00697
C16 H19 O6 Cl1	341.07974
C14 H13 O8 Cl1	343.02262
C14 H15 O8 Cl1	345.03827
C14 H17 O8 Cl1	347.05392
C13 H14 O7 Cl2	351.00439
C16 H15 O7 Cl1	353.04336
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C15 H15 O8 Cl1	357.03827
C14 H16 O7 Cl2	365.02004
C16 H15 O8 Cl1	369.03827
C15 H13 O9 Cl1	371.01754
C16 H17 O8 Cl1	371.05392
C15 H15 O9 Cl1	373.03319
C14 H12 O8 Cl2	376.98365
C18 H19 O7 Cl1	381.07466
C16 H15 O9 Cl1	385.03319
C15 H14 O8 Cl2	390.99930
C14 H12 O9 Cl2	392.97857
C15 H16 O8 Cl2	393.01495
C14 H14 O9 Cl2	394.99422
C17 H17 O9 Cl1	399.04884
C16 H15 O10 Cl1	401.02810
C16 H17 O10 Cl1	403.04375
C15 H12 O9 Cl2	404.97857
C15 H14 O9 Cl2	406.99422
C16 H18 O8 Cl2	407.03060
C15 H16 O9 Cl2	409.00987
C18 H19 O9 Cl1	413.06449
C17 H17 O10 Cl1	415.04375
C19 H19 O9 Cl1	425.06449

DWTP1+DWTP4 (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C18 H17 O10 Cl1	427.04375
C19 H25 O9 Cl1	431.11144
C17 H16 O9 Cl2	433.00987
C18 H17 O11 Cl1	443.03867
C19 H23 O10 Cl1	445.09070
C18 H20 O9 Cl2	449.04117
C18 H18 O10 Cl2	463.02043
C33 H28 O6 Cl4	659.05673

Table S21. List of verified formulae of the 80 DBPs common to DWTP2 and DWTP3 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP2+DWTP3	
Molecular formula	***Theoretical mass of the negative ion***
C12 H11 O6 Cl1	285.01714
C13 H15 O5 Cl1	285.05353
C12 H13 O6 Cl1	287.03279
C14 H13 O5 Cl1	295.03788
C14 H15 O5 Cl1	297.05353
C13 H13 O6 Cl1	299.03279
C12 H11 O7 Cl1	301.01206
C13 H15 O6 Cl1	301.04844
C14 H19 O5 Cl1	301.08483
C12 H13 O7 Cl1	303.02771
C13 H19 O6 Cl1	305.07974
C14 H9 O6 Cl1	307.00149
C15 H15 O5 Cl1	309.05353
C14 H13 O6 Cl1	311.03279
C15 H17 O5 Cl1	311.06918
C13 H11 O7 Cl1	313.01206
C15 H19 O5 Cl1	313.08483
C13 H13 O7 Cl1	315.02771
C13 H15 O7 Cl1	317.04336
C15 H13 O6 Cl1	323.03279
C14 H11 O7 Cl1	325.01206
C15 H15 O6 Cl1	325.04844
C14 H13 O7 Cl1	327.02771
C15 H17 O6 Cl1	327.06409
C13 H11 O8 Cl1	329.00697
C16 H23 O5 Cl1	329.11613
C13 H13 O8 Cl1	331.02262
C14 H17 O7 Cl1	331.05901
C15 H11 O7 Cl1	337.01206
C16 H15 O6 Cl1	337.04844
C17 H19 O5 Cl1	337.08483
C15 H13 O7 Cl1	339.02771
C16 H17 O6 Cl1	339.06409
C14 H11 O8 Cl1	341.00697
C14 H13 O8 Cl1	343.02262
C14 H15 O8 Cl1	345.03827
C16 H13 O7 Cl1	351.02771
C15 H11 O8 Cl1	353.00697
C16 H15 O7 Cl1	353.04336
C17 H19 O6 Cl1	353.07974

DWTP2+DWTP3 (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C14 H13 O6 Br1	354.98228
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C17 H21 O6 Cl1	355.09539
C15 H15 O8 Cl1	357.03827
C15 H17 O8 Cl1	359.05392
C15 H19 O8 Cl1	361.06957
C16 H23 O7 Cl1	361.10596
C17 H17 O7 Cl1	367.05901
C18 H21 O6 Cl1	367.09539
C16 H15 O8 Cl1	369.03827
C17 H19 O7 Cl1	369.07466
C15 H13 O9 Cl1	371.01754
C16 H19 O8 Cl1	373.06957
C16 H21 O8 Cl1	375.08522
C17 H15 O8 Cl1	381.03827
C18 H19 O7 Cl1	381.07466
C17 H17 O8 Cl1	383.05392
C19 H25 O6 Cl1	383.12669
C16 H15 O9 Cl1	385.03319
C17 H19 O8 Cl1	385.06957
C16 H17 O9 Cl1	387.04884
C17 H23 O8 Cl1	389.10087
C17 H19 O6 Br1	397.02923
C18 H19 O8 Cl1	397.06957
C19 H23 O7 Cl1	397.10596
C17 H17 O9 Cl1	399.04884
C20 H29 O6 Cl1	399.15799
C17 H19 O9 Cl1	401.06449
C17 H23 O9 Cl1	405.09579
C18 H27 O8 Cl1	405.13217
C18 H19 O9 Cl1	413.06449
C18 H21 O9 Cl1	415.08014
C17 H19 O10 Cl1	417.0594
C20 H21 O9 Cl1	439.08014
C18 H15 O11 Cl1	441.02302
C20 H23 O9 Cl1	441.09579
C21 H27 O8 Cl1	441.13217
C19 H21 O10 Cl1	443.07505
C20 H25 O9 Cl1	443.11144

Table S22. List of verified formulae of the 190 DBPs common to DWTP2 and DWTP4 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP2+DWTP4 (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C12 H13 O4 Cl1	255.04296
C5 H1 O3 Cl2 Br1	256.84134
C11 H13 O5 Cl1	259.03788
C11 H7 O6 Cl1	268.98584
C12 H11 O5 Cl1	269.02223
C13 H15 O4 Cl1	269.05861
C11 H9 O6 Cl1	271.00149
C12 H13 O5 Cl1	271.03788
C11 H11 O6 Cl1	273.01714
C12 H15 O5 Cl1	273.05353
C11 H15 O6 Cl1	277.04844
C12 H9 O6 Cl1	283.00149
C12 H11 O6 Cl1	285.01714
C12 H13 O6 Cl1	287.03279
C13 H17 O5 Cl1	287.06918
C11 H8 O5 Cl2	288.96761
C11 H11 O7 Cl1	289.01206
C12 H15 O6 Cl1	289.04844
C11 H13 O7 Cl1	291.02771
C11 H12 O5 Cl2	292.99891
C10 H10 O6 Cl2	294.97817
C13 H9 O6 Cl1	295.00149
C14 H13 O5 Cl1	295.03788
C10 H12 O6 Cl2	296.99382
C13 H11 O6 Cl1	297.01714
C12 H9 O7 Cl1	298.99641
C12 H11 O7 Cl1	301.01206
C12 H13 O7 Cl1	303.02771
C11 H8 O6 Cl2	304.96252
C12 H15 O7 Cl1	305.04336
C13 H19 O6 Cl1	305.07974
C11 H10 O6 Cl2	306.97817
C12 H14 O5 Cl2	307.01456
C10 H8 O7 Cl2	308.95744
C11 H12 O6 Cl2	308.99382
C14 H11 O6 Cl1	309.01714
C15 H15 O5 Cl1	309.05353
C10 H10 O7 Cl2	310.97309
C13 H9 O7 Cl1	310.99641

DWTP2+DWTP4 (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C11 H14 O6 Cl2	311.00947
C14 H13 O6 Cl1	311.03279
C10 H12 O7 Cl2	312.98874
C13 H11 O7 Cl1	313.01206
C15 H19 O5 Cl1	313.08483
C13 H13 O7 Cl1	315.02771
C15 H21 O5 Cl1	315.10048
C12 H8 O6 Cl2	316.96252
C13 H12 O5 Cl2	316.99891
C13 H15 O7 Cl1	317.04336
C11 H6 O7 Cl2	318.94179
C12 H10 O6 Cl2	318.97817
C12 H13 O8 Cl1	319.02262
C13 H17 O7 Cl1	319.05901
C14 H21 O6 Cl1	319.09539
C11 H8 O7 Cl2	320.95744
C12 H12 O6 Cl2	320.99382
C12 H15 O8 Cl1	321.03827
C13 H19 O7 Cl1	321.07466
C11 H10 O7 Cl2	322.97309
C14 H9 O7 Cl1	322.99641
C12 H14 O6 Cl2	323.00947
C15 H13 O6 Cl1	323.03279
C16 H17 O5 Cl1	323.06918
C11 H12 O7 Cl2	324.98874
C14 H11 O7 Cl1	325.01206
C15 H15 O6 Cl1	325.04844
C11 H14 O7 Cl2	327.00439
C14 H13 O7 Cl1	327.02771
C15 H17 O6 Cl1	327.06409
C13 H11 O8 Cl1	329.00697
C15 H19 O6 Cl1	329.07974
C16 H23 O5 Cl1	329.11613
C13 H10 O6 Cl2	330.97817
C13 H13 O8 Cl1	331.02262
C16 H25 O5 Cl1	331.13178
C12 H8 O7 Cl2	332.95744
C13 H12 O6 Cl2	332.99382
C13 H15 O8 Cl1	333.03827

Table S24. (cont.)

DWTP2+DWTP4 (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C12 H10 O7 Cl2	334.97309
C13 H14 O6 Cl2	335.00947
C13 H17 O8 Cl1	335.05392
C12 H12 O7 Cl2	336.98874
C15 H11 O7 Cl1	337.01206
C13 H16 O6 Cl2	337.02512
C16 H15 O6 Cl1	337.04844
C11 H10 O8 Cl2	338.96800
C12 H14 O7 Cl2	339.00439
C15 H13 O7 Cl1	339.02771
C11 H12 O8 Cl2	340.98365
C14 H11 O8 Cl1	341.00697
C14 H13 O8 Cl1	343.02262
C13 H11 O9 Cl1	345.00189
C14 H15 O8 Cl1	345.03827
C17 H27 O5 Cl1	345.14743
C13 H10 O7 Cl2	346.97309
C14 H14 O6 Cl2	347.00947
C14 H17 O8 Cl1	347.05392
C13 H12 O7 Cl2	348.98874
C12 H10 O8 Cl2	350.96800
C13 H14 O7 Cl2	351.00439
C16 H13 O7 Cl1	351.02771
C14 H18 O6 Cl2	351.04077
C17 H17 O6 Cl1	351.06409
C12 H12 O8 Cl2	352.98365
C15 H11 O8 Cl1	353.00697
C13 H16 O7 Cl2	353.02004
C16 H15 O7 Cl1	353.04336
C12 H14 O8 Cl2	354.99930
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C18 H25 O5 Cl1	355.13178
C14 H11 O9 Cl1	357.00189
C15 H15 O8 Cl1	357.03827
C18 H27 O5 Cl1	357.14743
C14 H10 O7 Cl2	358.97309
C14 H13 O9 Cl1	359.01754
C13 H8 O8 Cl2	360.95235
C14 H12 O7 Cl2	360.98874

DWTP2+DWTP4 (continued)	
Molecular formula	***Theoretical mass of te negative ion***
C15 H16 O6 Cl2	361.02512
C14 H15 O9 Cl1	361.03319
C15 H19 O8 Cl1	361.06957
C14 H14 O7 Cl2	363.00439
C15 H18 O6 Cl2	363.04077
C13 H12 O8 Cl2	364.98365
C14 H16 O7 Cl2	365.02004
C13 H14 O8 Cl2	366.99930
C14 H18 O7 Cl2	367.03569
C17 H17 O7 Cl1	367.05901
C12 H12 O9 Cl2	368.97857
C15 H11 O9 Cl1	369.00189
C13 H16 O8 Cl2	369.01495
C16 H15 O8 Cl1	369.03827
C19 H27 O5 Cl1	369.14743
C15 H13 O9 Cl1	371.01754
C19 H29 O5 Cl1	371.16308
C15 H12 O7 Cl2	372.98874
C15 H15 O9 Cl1	373.03319
C14 H10 O8 Cl2	374.96800
C15 H17 O9 Cl1	375.04884
C14 H12 O8 Cl2	376.98365
C15 H16 O7 Cl2	377.02004
C15 H19 O9 Cl1	377.06449
C14 H14 O8 Cl2	378.99930
C15 H18 O7 Cl2	379.03569
C13 H12 O9 Cl2	380.97857
C14 H16 O8 Cl2	381.01495
C17 H15 O8 Cl1	381.03827
C18 H19 O7 Cl1	381.07466
C13 H14 O9 Cl2	382.99422
C16 H13 O9 Cl1	383.01754
C14 H18 O8 Cl2	383.03060
C16 H15 O9 Cl1	385.03319
C15 H12 O8 Cl2	388.98365
C16 H19 O9 Cl1	389.06449
C18 H27 O7 Cl1	389.13726
C14 H10 O9 Cl2	390.96292
C15 H14 O8 Cl2	390.99930
C16 H18 O7 Cl2	391.03569

Table S24. (cont.)

DWTP2+DWTP4 (continued)	
Molecular formula	***Theoretical mass of the negative ion***
C14 H12 O9 Cl2	392.97857
C15 H16 O8 Cl2	393.01495
C14 H14 O9 Cl2	394.99422
C14 H16 O9 Cl2	397.00987
C17 H15 O9 Cl1	397.03319
C18 H19 O8 Cl1	397.06957
C20 H27 O6 Cl1	397.14234
C16 H13 O10 Cl1	399.01245
C17 H17 O9 Cl1	399.04884
C16 H15 O10 Cl1	401.02810
C16 H32 O4 Cl1 Br1	401.10998
C15 H10 O9 Cl2	402.96292
C16 H14 O8 Cl2	402.99930
C16 H17 O10 Cl1	403.04375
C19 H29 O7 Cl1	403.15291
C15 H12 O9 Cl2	404.97857
C16 H16 O8 Cl2	405.01495
C16 H18 O8 Cl2	407.03060
C18 H19 O9 Cl1	413.06449
C17 H17 O10 Cl1	415.04375
C17 H19 O10 Cl1	417.05940
C15 H12 O10 Cl2	420.97348
C19 H19 O9 Cl1	425.06449
C18 H19 O10 Cl1	429.05940
C19 H27 O9 Cl1	433.12709
C20 H21 O9 Cl1	439.08014
C21 H27 O8 Cl1	441.13217
C21 H31 O8 Cl1	445.16347
C19 H25 O10 Cl1	447.10635
C20 H21 O10 Cl1	455.07505
C20 H23 O11 Cl1	473.08562
C25 H31 O12 Cl1	557.14313

Table S23. List of verified formulae of the 61 DBPs common to DWTP3 and DWTP4 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP3+DWTP4	
Molecular formula	***Theoretical mass of the negative ion***
C13 H13 O5 Cl1	283.03788
C12 H11 O6 Cl1	285.01714
C12 H13 O6 Cl1	287.03279
C14 H13 O5 Cl1	295.03788
C12 H11 O7 Cl1	301.01206
C12 H13 O7 Cl1	303.02771
C13 H19 O6 Cl1	305.07974
C15 H15 O5 Cl1	309.05353
C14 H13 O6 Cl1	311.03279
C13 H11 O7 Cl1	313.01206
C15 H19 O5 Cl1	313.08483
C13 H13 O7 Cl1	315.02771
C13 H15 O7 Cl1	317.04336
C15 H13 O6 Cl1	323.03279
C14 H11 O7 Cl1	325.01206
C15 H15 O6 Cl1	325.04844
C14 H13 O7 Cl1	327.02771
C15 H17 O6 Cl1	327.06409
C13 H11 O8 Cl1	329.00697
C16 H23 O5 Cl1	329.11613
C13 H13 O8 Cl1	331.02262
C15 H11 O7 Cl1	337.01206
C16 H15 O6 Cl1	337.04844
C15 H13 O7 Cl1	339.02771
C14 H11 O8 Cl1	341.00697
C14 H13 O8 Cl1	343.02262
C14 H15 O8 Cl1	345.03827
C16 H13 O7 Cl1	351.02771
C15 H11 O8 Cl1	353.00697
C16 H15 O7 Cl1	353.04336
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C15 H15 O8 Cl1	357.03827
C15 H19 O8 Cl1	361.06957
C17 H15 O7 Cl1	365.04336
C18 H19 O6 Cl1	365.07974
C17 H17 O7 Cl1	367.05901

DWTP3+DWTP4	
Molecular formula	***Theoretical mass of the negative ion***
C16 H15 O8 Cl1	369.03827
C15 H13 O9 Cl1	371.01754
C16 H17 O8 Cl1	371.05392
C18 H17 O7 Cl1	379.05901
C17 H15 O8 Cl1	381.03827
C18 H19 O7 Cl1	381.07466
C19 H23 O6 Cl1	381.11104
C16 H15 O9 Cl1	385.03319
C18 H17 O8 Cl1	395.05392
C18 H19 O8 Cl1	397.06957
C17 H17 O9 Cl1	399.04884
C18 H17 O9 Cl1	411.04884
C19 H21 O8 Cl1	411.08522
C18 H19 O9 Cl1	413.06449
C17 H19 O10 Cl1	417.05940
C18 H17 O10 Cl1	427.04375
C19 H21 O9 Cl1	427.08014
C20 H25 O8 Cl1	427.11652
C18 H21 O10 Cl1	431.07505
C19 H25 O9 Cl1	431.11144
C19 H17 O10 Cl1	439.04375
C20 H21 O9 Cl1	439.08014
C21 H27 O8 Cl1	441.13217
C19 H23 O10 Cl1	445.09070
C16 H17 O8 Cl1	371.05392

Table S24. List of verified formulae of the 33 DBPs common to DWTP1, DWTP2, and DWTP3 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP1+DWTP2+DWTP3	
Molecular formula	***Theoretical mass of the negative ion***
C13 H13 O6 Cl1	299.03279
C13 H15 O6 Cl1	301.04844
C14 H13 O6 Cl1	311.03279
C15 H17 O5 Cl1	311.06918
C13 H11 O7 Cl1	313.01206
C13 H13 O7 Cl1	315.02771
C13 H15 O7 Cl1	317.04336
C14 H13 O7 Cl1	327.02771
C13 H13 O8 Cl1	331.02262
C16 H17 O6 Cl1	339.06409
C14 H11 O8 Cl1	341.00697
C14 H13 O8 Cl1	343.02262
C14 H15 O8 Cl1	345.03827
C16 H15 O7 Cl1	353.04336
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C15 H15 O8 Cl1	357.03827
C15 H17 O8 Cl1	359.05392
C16 H15 O8 Cl1	369.03827
C17 H19 O7 Cl1	369.07466
C15 H13 O9 Cl1	371.01754
C16 H19 O8 Cl1	373.06957
C16 H21 O8 Cl1	375.08522
C18 H19 O7 Cl1	381.07466
C17 H17 O8 Cl1	383.05392
C16 H15 O9 Cl1	385.03319
C17 H19 O8 Cl1	385.06957
C16 H17 O9 Cl1	387.04884
C17 H17 O9 Cl1	399.04884
C17 H19 O9 Cl1	401.06449
C18 H19 O9 Cl1	413.06449
C20 H23 O9 Cl1	441.09579
C19 H21 O10 Cl1	443.07505

Table S25. List of verified formulae of the 23 DBPs common to DWTP1, DWTP3, and DWTP4 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP1+DWTP3+DWTP4	
Molecular formula	***Theoretical mass of the negative ion***
C14 H13 O6 Cl1	311.03279
C13 H11 O7 Cl1	313.01206
C13 H13 O7 Cl1	315.02771
C13 H15 O7 Cl1	317.04336
C14 H13 O7 Cl1	327.02771
C13 H13 O8 Cl1	331.02262
C14 H11 O8 Cl1	341.00697
C14 H13 O8 Cl1	343.02262
C14 H15 O8 Cl1	345.03827
C16 H15 O7 Cl1	353.04336
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C15 H15 O8 Cl1	357.03827
C16 H15 O8 Cl1	369.03827
C15 H13 O9 Cl1	371.01754
C16 H17 O8 Cl1	371.05392
C18 H19 O7 Cl1	381.07466
C16 H15 O9 Cl1	385.03319
C17 H17 O9 Cl1	399.04884
C18 H19 O9 Cl1	413.06449
C18 H17 O10 Cl1	427.04375
C19 H25 O9 Cl1	431.11144
C19 H23 O10 Cl1	445.09070

Table S26. List of verified formulae of the 45 DBPs common to DWTP2, DWTP3, and DWTP4 according to negative ESI-FT-ICR MS analysis (only present in all three replicates of disinfected water).

DWTP2+DWTP3+DWTP4	
Molecular formula	***Theoretical mass of the negative ion***
C12 H11 O6 Cl1	285.01714
C12 H13 O6 Cl1	287.03279
C14 H13 O5 Cl1	295.03788
C12 H11 O7 Cl1	301.01206
C12 H13 O7 Cl1	303.02771
C13 H19 O6 Cl1	305.07974
C15 H15 O5 Cl1	309.05353
C14 H13 O6 Cl1	311.03279
C13 H11 O7 Cl1	313.01206
C15 H19 O5 Cl1	313.08483
C13 H13 O7 Cl1	315.02771
C13 H15 O7 Cl1	317.04336
C15 H13 O6 Cl1	323.03279
C14 H11 O7 Cl1	325.01206
C15 H15 O6 Cl1	325.04844
C14 H13 O7 Cl1	327.02771
C15 H17 O6 Cl1	327.06409
C13 H11 O8 Cl1	329.00697
C16 H23 O5 Cl1	329.11613
C13 H13 O8 Cl1	331.02262
C15 H11 O7 Cl1	337.01206
C16 H15 O6 Cl1	337.04844
C15 H13 O7 Cl1	339.02771
C14 H11 O8 Cl1	341.00697
C14 H13 O8 Cl1	343.02262
C14 H15 O8 Cl1	345.03827
C16 H13 O7 Cl1	351.02771
C15 H11 O8 Cl1	353.00697
C16 H15 O7 Cl1	353.04336
C15 H13 O8 Cl1	355.02262
C16 H17 O7 Cl1	355.05901
C15 H15 O8 Cl1	357.03827
C15 H19 O8 Cl1	361.06957
C17 H17 O7 Cl1	367.05901
C16 H15 O8 Cl1	369.03827
C15 H13 O9 Cl1	371.01754
C17 H15 O8 Cl1	381.03827

DWTP2+DWTP3+DWTP4 (cont.)	
Molecular formula	***Theoretical mass of the negative ion***
C18 H19 O7 Cl1	381.07466
C16 H15 O9 Cl1	385.03319
C18 H19 O8 Cl1	397.06957
C17 H17 O9 Cl1	399.04884
C18 H19 O9 Cl1	413.06449
C17 H19 O10 Cl1	417.0594
C20 H21 O9 Cl1	439.08014
C21 H27 O8 Cl1	441.13217

IX. Identification of DBPs in the investigated mixtures through LC-ESI(-)-Orbitrap MS

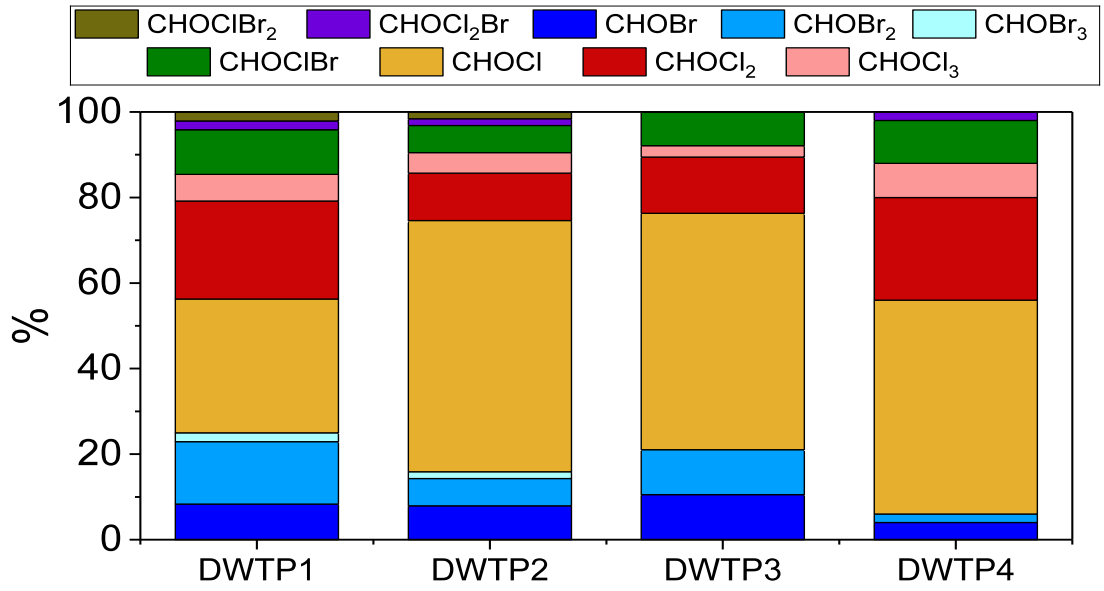


Figure S12. Contribution of each group of halogenated compounds to the chemodiversity of the investigated disinfected waters, after LC-ESI(-)-Orbitrap MS analysis. Y-axis shows the percent of confirmed or tentatively identified structures.

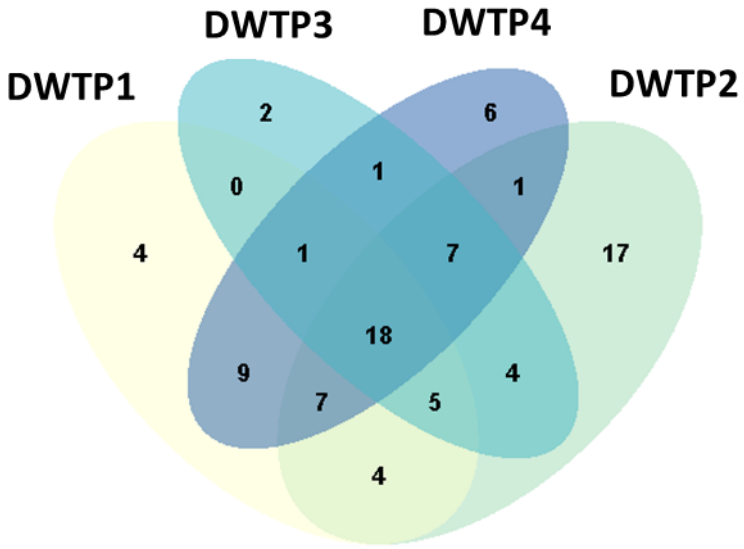


Figure S13. Venn diagram showing the chemodiversity of the investigated DBP mixtures according to LC-ESI(-)-Orbitrap MS analysis.

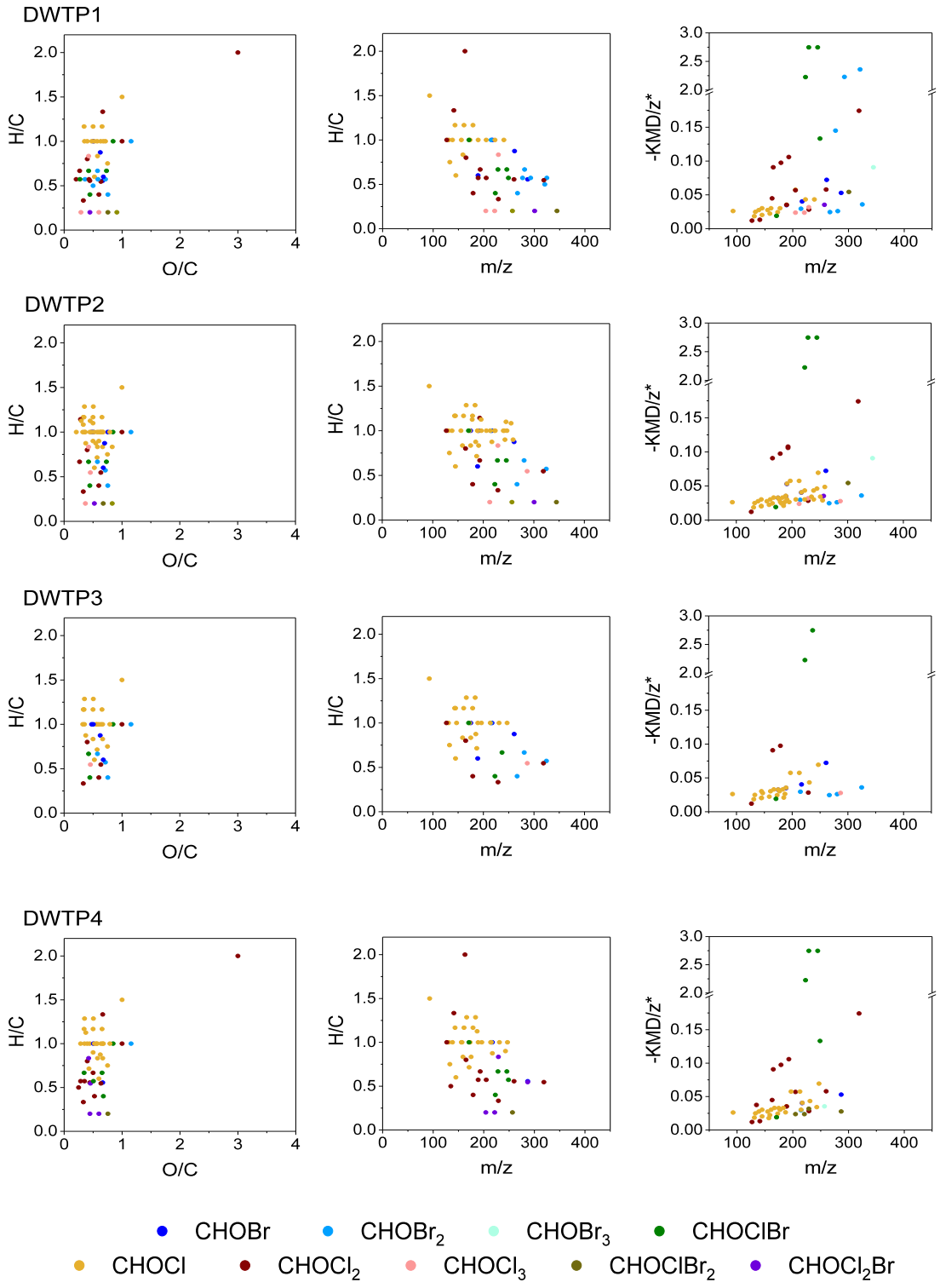


Figure S14. Molecular composition of the DBPs of each DWTP according to LC-ESI(-)-Orbitrap MS analysis, visualized by van Krevelen diagrams (left panel), mass edited H/C ratios (middle panel), and modified Kendrick mass defect plots (right panel). Only formulae present in all three replicates are shown.

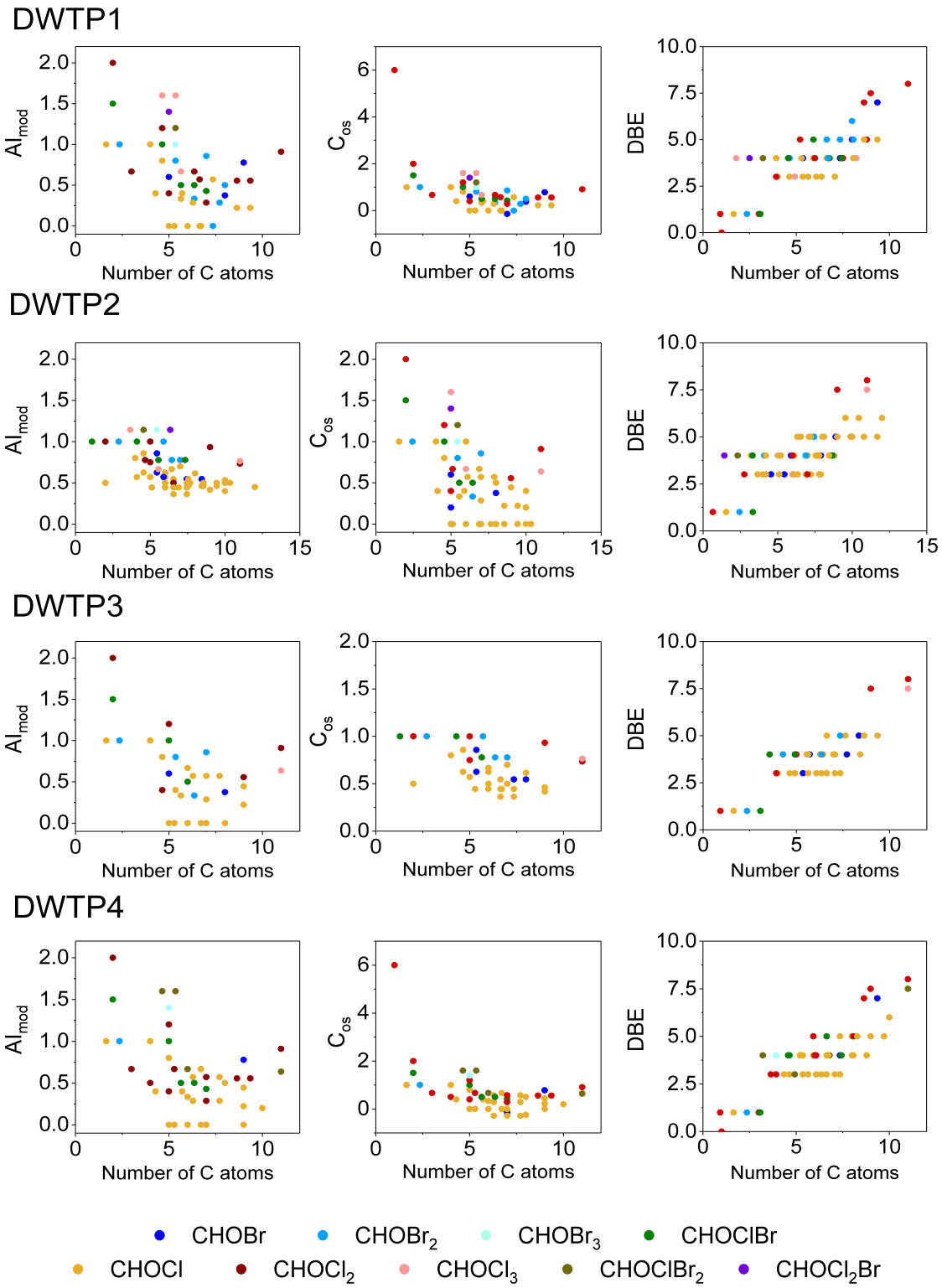


Figure S15. Plots showing DBE, AI_{mod}, and C_{OS} versus the number of carbon of DBPs (*m/z* ions only present in disinfected water) according to LC-ESI(-)-Orbitrap MS analysis.

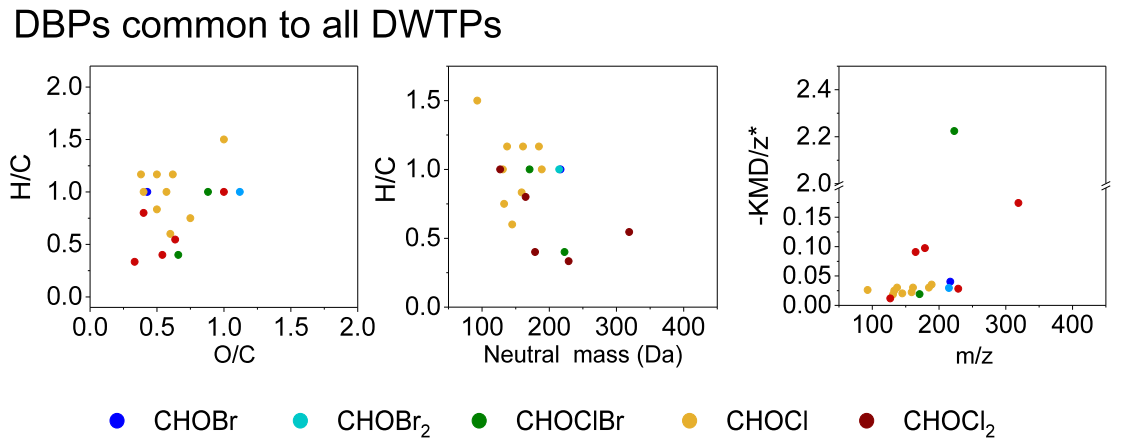


Figure S16. Molecular composition of the DBPs formed in all DWTPs according to LC-ESI(-)-Orbitrap MS analysis. van Krevelen diagrams (left panel), mass edited H/C ratios (middle panel), and modified Kendrick mass defect plots (right panel) of the compounds present in the disinfected samples. Only formulae present in the three replicates are shown.

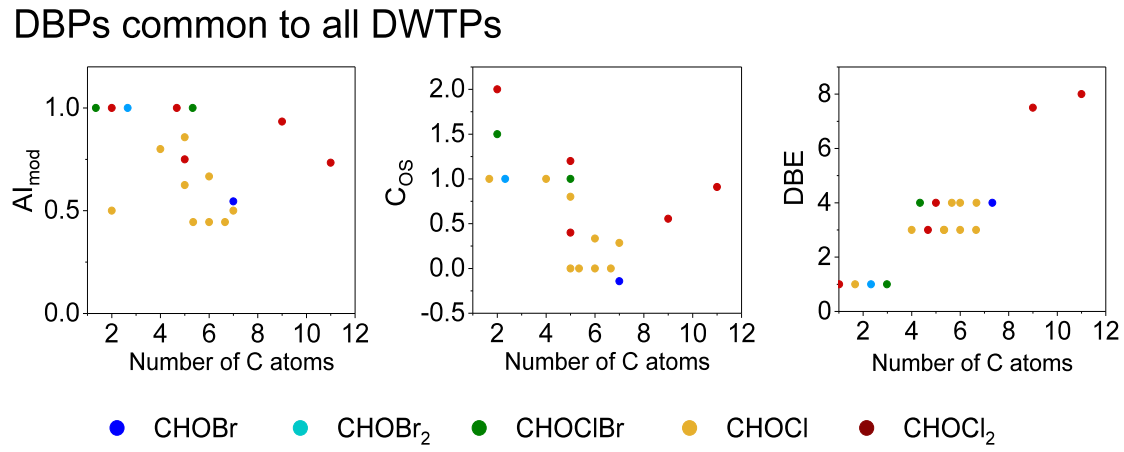


Figure S17. Plots showing DBE, AI_{mod}, and C_{OS} versus the number of carbon for verified DBPs (*m/z* ions only present in disinfected water) common to all DWTPs according to LC-ESI(-)-Orbitrap MS analysis.

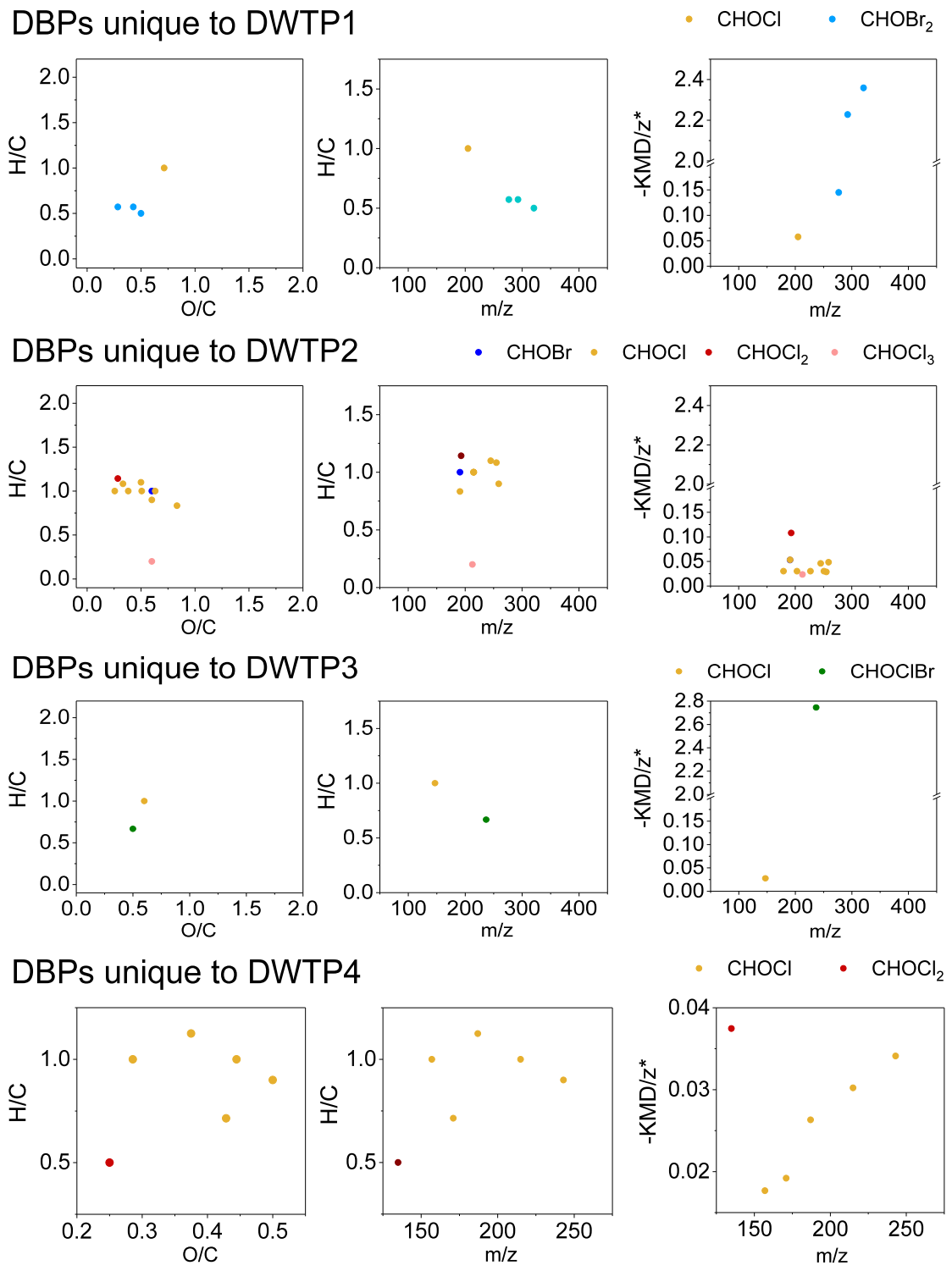


Figure S18. Molecular composition of unique DBPs according to LC-ESI(-)-Orbitrap MS analysis. van Krevelen diagrams (left panel), mass edited H/C ratios (middle panel), and modified Kendrick mass defect plots(right panel) of the compounds present in the disinfected samples. Only formulas present in the three replicates are shown.

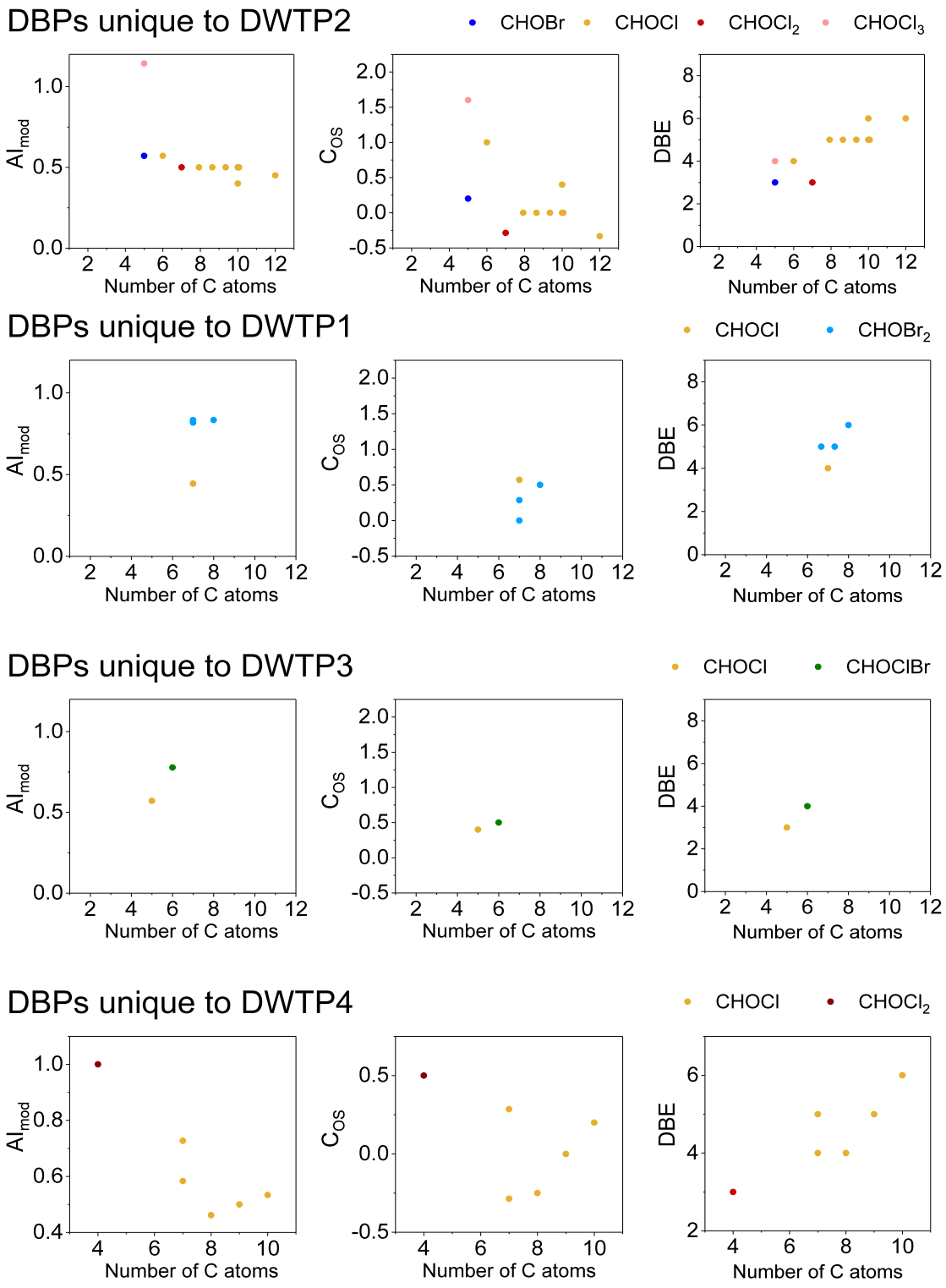
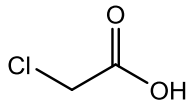
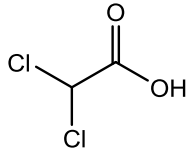
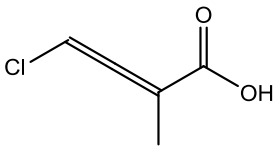
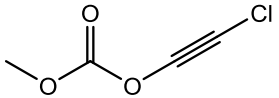
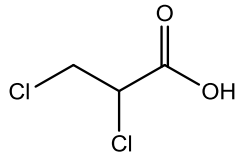
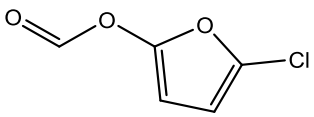
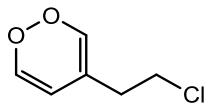
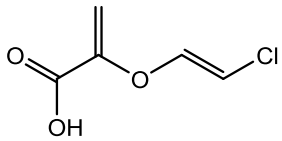
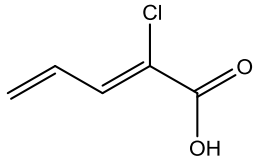
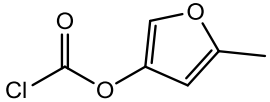
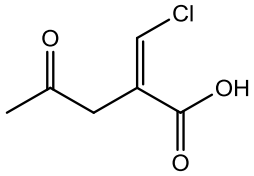


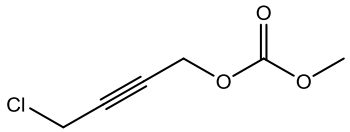
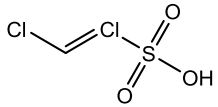
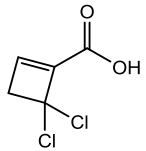
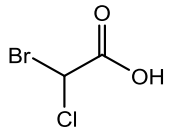
Figure S19. Plots showing DBE, AI_{mod}, and C_{OS} versus the number of carbon for verified DBPs (*m/z* ions only present in disinfected water) in unique DBPs according to LC-ESI(-)-Orbitrap MS analysis.

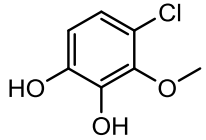
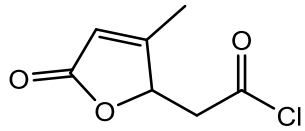
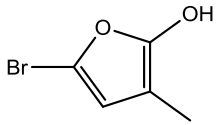
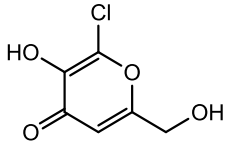
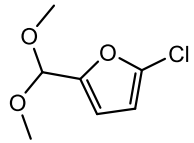
Table S27. DBPs identified after LC-ESI(-)MS/MS analyses with QExactive MS.

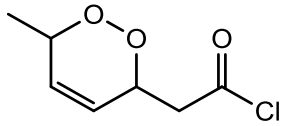
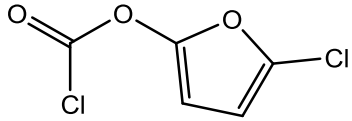
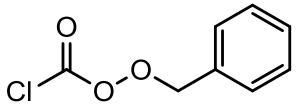
Parent ion				Presence in extracts					Suspect DBP (Level of confidence)	Identification evidence
Theor. mass [M-H]-	Elemental comp [M]	RDBE	Δ error (ppm)	Rt (min)	DW TP1	DW TP2	DW TP3	DW TP4		
92.9751	$C_2H_3ClO_2$	1.5	3.438	7.95	√	√	T	√	 *2-chloroacetic acid (*CL 1)	- Isotopic pattern of Cl - CONFIRMED with analytical standard
126.9359	$C_2H_2Cl_2O_2$	1.5	2.067	6.9	√√	√√√	√√	√√√	 *2,2-dichloroacetic acid (*CL 1)	- Isotopic pattern of Cl_2 - Characteristic fragments: 126.9361 ($C_2HCl_2O_2$) 82.9462 ($CHCl_2$) - The highest score in MetFrag - CONFIRMED with analytical standard
130.9905	$C_5H_5ClO_2$	3.5	2.287	9.73	√	√√	√√	√	 *4-chloro-2-methyl-buta-2,3-dienoic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 130.9908 ($C_5H_4ClO_2$) 113.0247 ($C_5H_5O_3$) 95.0140 ($C_5H_3O_2$) 87.0453 ($C_4H_7O_2$) - The highest score in MetFrag
132.9698	$C_4H_3ClO_3$	3.5	2.595	7.82	√	√√√	√√	√	 *chloroethynyl methyl carbonate* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 132.9701 ($C_4H_2ClO_3$) 74.9643 (C_2ClO) 68.9982 (C_3H_2O) 58.9692 (C_2Cl) - The highest score in MetFrag

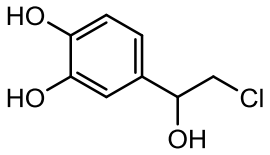
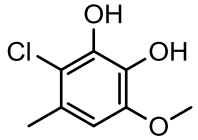
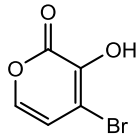
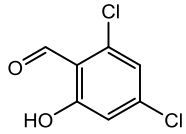
134.9413	$C_4H_2Cl_2O$	3.5	2.124	14.1	x	x	x	√	n/a (CL5)	- Isotopic pattern of Cl_2 - No MS2 available
140.9518	$C_3H_4Cl_2O_2$	1.5	2.851	13.1	√	x	x	√√	 *2,3-dichloropropanoic acid* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 140.9520 ($C_3H_3Cl_2O_2$) 104.9751 ($C_3H_2ClO_2$) 96.9617 ($C_2H_3Cl_2$) 71.0139 ($C_3H_3O_2$) - The highest score in MetFrag
144.9698	$C_5H_3ClO_3$	4.5	1.414	6.85	√√	√√√	√√	√√	 *5-chlorofuran-2-yl formate* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 144.9700 ($C_5H_2ClO_3$) 116.9799 ($C_4H_2ClO_2$) 100.9799 (C_4H_2ClO) 74.9643 (C_2ClO) 65.0032 (C_4HO) - The highest score in MetFrag
145.0065	$C_6H_7ClO_2$	3.5	2.066	11.7	X	√√	√	x	 *4-(2-chloroethyl)-1,2-dioxine* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 145.0065 ($C_6H_6ClO_2$) 83.0143 ($C_4H_3O_2$) 81.0143 (C_5H_5O) - The highest score in MetFrag
146.9854	$C_5H_5ClO_3$	3.5	2.483	9.5	√	√√√	√√	√	 *2-((2-chlorovinyl)oxy)acrylic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 146.9857 ($C_5H_4ClO_3$) 102.9958 (C_4H_4ClO) 67.0189 (C_4H_3O) 58.9692 (C_2Cl) - The highest score in MetFrag

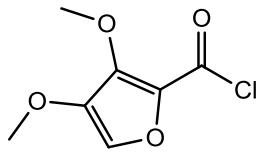
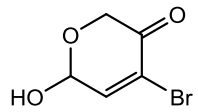
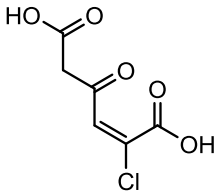
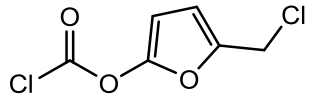
146.9854	$C_5H_5ClO_3$	3.5	1.829	5.47	√	√	x	√	 *2-chloropenta-2,4-dienoic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 146.9857 ($C_5H_4ClO_3$) 104.9753 ($C_3H_2ClO_2$) 67.0189 (C_4H_3O) 58.9692 (C_2Cl) - The highest score in MetFrag
157.0063	$C_7H_7ClO_2$	4.5	0.952	13.1	x	x	x	√	n/a (CL 4)	- Isotopic pattern of Cl - No MS2 available
158.9857	$C_6H_5ClO_3$	4.5	1.101	9.23	X	√√	√	√	 *(5-methyl-3-furyl) carbonochloridate* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 158.9857 ($C_6H_4ClO_3$) 143.9623 (C_5HClO_3) 130.9544 (C_4ClO_3) 114.9960 (C_5H_4ClO) 79.0190 (C_5H_3O) 83.0140 ($C_4H_3O_2$) - The highest score in MetFrag
161.0012	$C_6H_7ClO_3$	3.5	0.776	8.38	T	√√	√	√	 *2-(chloromethylene)-4-oxo-pentanoic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 161.0012 ($C_6H_6ClO_3$) 118.9906 ($C_4H_4ClO_2$) 125.0245 ($C_6H_5O_3$) 83.0140 (C_4H_3O) 57.0342 (C_3H_5O) - The highest score in MetFrag

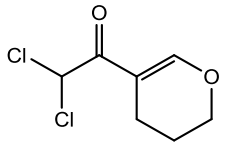
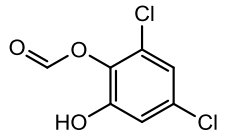
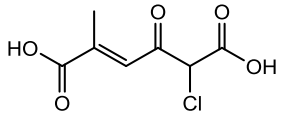
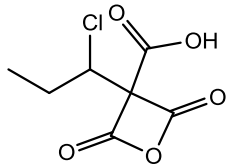
161.0012	$C_6H_7ClO_3$	3.5	0.776	8.8	T	√√	√	√	 *4-chlorobut-2-ynyl methyl carbonate* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 160.0012 ($C_6H_6ClO_3$) 128.9751 ($C_5H_2ClO_2$) 110.0011 ($C_5H_2O_3$) 95.0141 ($C_5H_3O_2$) 72.9930 (C_2HO_3) - The highest score in MetFrag
161.0012	$C_6H_7ClO_3$	3.5	0.776	11.8	T	√√	T	T	n/a (CL 4)	- Isotopic pattern of Cl - No MS2 available
162.9032	$CH_2Cl_2O_3S$	0.5	2.067	6.24	√	x	x	√√	 *Chloro-(sulfoλ3-chloranylidene)methane* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 162.9032 ($CHCl_2O_3S$) 98.9315 (O_2ClS) 79.9575 (O_3S) - The highest score in MetFrag
164.9517	$C_5H_4Cl_2O_2$	3.5	0.678	8.79	√	√√	√	√	 *4,4-dichlorocyclobutene-1-carboxylic acid* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 164.9516 ($C_5H_3Cl_2O_2$) 128.9751 ($C_5H_2ClO_2$) 92.9982 (C_5HO_2) 96.9604 ($C_2H_3Cl_2$) - The highest score in MetFrag
170.8854	$C_2H_2BrClO_2$	1.5	1.621	8.05	√√	√√√	√√	√√√	 *2-bromo,2-chloroacetic acid* (CL 1)	- Isotopic pattern of BrCl - Characteristic fragments: 170.8855($C_2HBrClO_2$) 126.8958(CHBrCl) 78.9189 (Br) - Unique score in MetFrag - CONFIRMED with analytical std
170.9857	$C_7H_5ClO_3$	5.5	1.140	20.2	x	x	x	√	n/a (CL 4)	- Isotopic pattern of Cl - No MS2 available

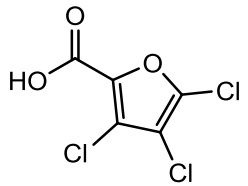
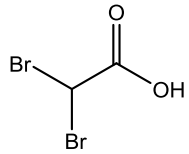
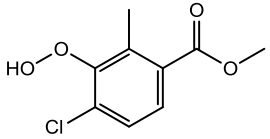
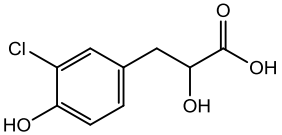
173.0011	$C_7H_7ClO_3$	4.5	1.184	9.6	x	√	x	x	 *4-chloro-3-methoxy-benzene-1,2-diol* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 173.0012($C_7H_6ClO_3$) 142.9907($C_6H_4ClO_2$) 111.0458 ($C_6H_7O_2$) 65.0032 (C_4HO) - -The highest score in MetFrag
173.0011	$C_7H_7ClO_3$	4.5	3.834	10.9	√	√√	x	√	 *2-(3-methyl-5-oxo-2H-furan-2-yl)acetyl chloride* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 173.0012 ($C_7H_6ClO_3$) 157.9778 ($C_6H_3ClO_3$) 129.298 ($C_6H_5O_2$) 97.0297 ($C_5H_5O_2$) - The highest score in MetFrag
174.9400	$C_5H_5BrO_2$	3.5	-0.259	10.2	x	√√	√√	x	 *5-bromo-3-methyl-furan-2-ol* (CL3)	- Isotopic pattern of Br - Characteristic fragments: 174.9401 ($C_5H_4BrO_2$) 95.0141 ($C_5H_3O_2$) 78.9189 (Br) - The highest score in MetFrag
174.9803	$C_6H_5ClO_4$	4.5	-0.284	7.15	x	√	x	√	 *2-chloro-3-hydroxy-6-(hydroxymethyl)pyran-4-one* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 174.9803 ($C_6H_4ClO_4$) 139.0037 ($C_6H_3O_4$) 111.0090 ($C_5H_3O_3$) 83.0139 ($C_4H_3O_2$) 67.0188 (C_4H_3O) - The highest score in MetFrag
175.0167	$C_7H_9ClO_3$	3.5	0.256	8.90	x	√√	√	√		- Isotopic pattern of Cl - Characteristic fragments: 173.0012 ($C_7H_8ClO_3$) 142.9906 ($C_6H_4ClO_2$)

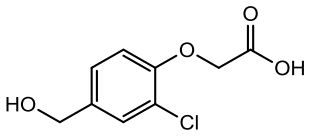
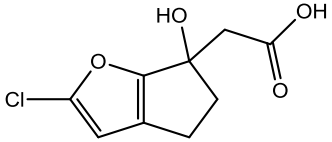
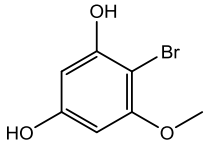
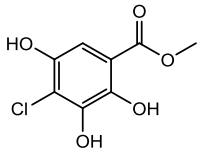
									2-chloro-5-(dimethoxymethyl)furan (CL 3)	109.0298 ($C_6H_5O_2$) 65.0032 (C_4HO) - The highest score in MetFrag
175.0167	$C_7H_9ClO_3$	3.5	0.256	9.26	x	√√	T	√	 *2-6-methyl-3,6-dihydro-1,2-dioxin-3-yl]acetyl chloride* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 175.0168 ($C_7H_8ClO_3$) 139.0403 ($C_7H_7O_3$) 111.0454 ($C_6H_7O_2$) 104.9750 ($C_3H_2ClO_2$) 83.0503 (C_5H_7O) 55.0185 (C_3H_3O) - -The highest score in MetFrag
178.9308	$C_5H_2Cl_2O_3$	4.5	2.668	9.5/ 11.45	√√	√√√	√√	√√	 *5-chlorofuran-2-yl carbonochloridate* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 178.9311 ($C_5HCl_2O_3$) 142.9546 (C_5ClO_3) 98.9646 (C_4ClO) 70.9694 (C_3ClO) -The highest score in MetFrag
185.0014	$C_8H_7ClO_3$	5.5	1.756	7.98	X	√	√	X	 *benzyloxy carbonochloridate* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 185.0015 ($C_8H_6ClO_3$) 149.0248 ($C_8H_5O_3$) 105.0348 (C_7H_5O) 81.0347 (C_5H_5O) 78.9592 ($CClO_2$) -The highest score in MetFrag
186.9802	$C_7H_5ClO_4$	5.5	-0.105	11.9	X	√	√	X	n/a (CL 4)	- Isotopic pattern of Cl - No MS2 available

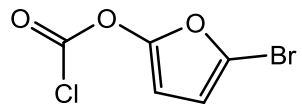
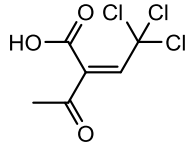
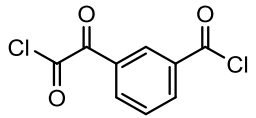
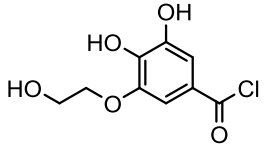
187.0168	$C_8H_9ClO_3$	4.5	0.400	9.7	x	√√	x	x	 *4-[2-chloro-1-hydroxy-ethyl]benzene-1,2-diol* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 187.0168 ($C_8H_8ClO_3$) 125.0611 ($C_7H_9ClO_2$) 109.0296 ($C_6H_5O_2$) 68.9981 (C_3HO_2) - The highest score in MetFrag
187.0168	$C_8H_9ClO_3$	4.5	0.293	10.8	x	√√	x	√	 *3-chloro-6-methoxy-4-methyl-benzene-1,2-dio* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 187.0168 ($C_8H_8ClO_3$) 157.0063 ($C_7H_6ClO_2$) 154.9907 ($C_7H_4ClO_2$) 121.0297 ($C_7H_5O_2$) 79.0190 (C_5H_3O) 65.0031 (C_4HO) - The highest score in MetFrag
188.9193	$C_5H_3BrO_3$	4.5	1.906	7.12	√	√√	√√	x	 4-bromo-3-hydroxy-pyran-2-one *(*CL:3)	- Isotopic pattern of Br - Characteristic fragments: 188.9195 ($C_5H_2BrO_3$) 87.0089 (C_3HO_3) 78.9190 (Br) 65.0033 (C_4HO) - -The highest score in MetFrag
188.9516	$C_7H_4Cl_2O_2$	5.5	1.545	19.0	√	x	x	T	 *2,4-dichloro-6-hydroxy-benzaldehyde* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 188.9520 ($C_7H_3Cl_2O_2$) - The highest score in MetFrag

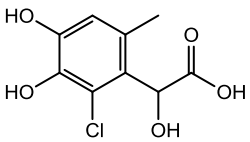
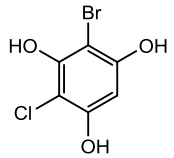
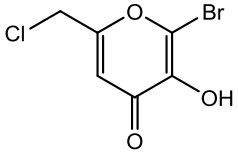
188.9963	$C_7H_7ClO_4$	4.5	0.901	8.82	√	√√	√	√	 *3,4-dimethoxyfuran-2-carbonyl chloride* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 188.9961 ($C_7H_6ClO_4$) 158.9854 ($C_6H_4ClO_3$) 144.9698 ($C_5H_2ClO_3$) 123.0089 ($C_6H_3O_3$) 95.0141 ($C_5H_3O_2$) 79.0190 (C_5H_3O) - The highest score in MetFrag
190.9352	$C_5H_5BrO_3$	3.5	1.048	9.76	x	√√	x	x	 *4-bromo-6-hydroxy-2H-pyran-3(6H)-one* (CL 3)	- Isotopic pattern of Br - Characteristic fragments: 190.9351 ($C_5H_4BrO_3$) 146.9450 (C_4H_4BrO) 102.9190 (C_2Br) 78.9190 (Br) 67.0188 (C_4H_3O) - The highest score in MetFrag
190.9751	$C_6H_5ClO_5$	4.5	-0.703	7.37	X	√√	x	x	 *(E)-2-chloro-4-oxo-hex-2-enedioic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 190.9751 ($C_6H_4ClO_5$) 146.9856 ($C_5H_4ClO_3$) 111.0090 ($C_5H_3O_3$) 83.0139 ($C_4H_3O_2$) 67.0188 (C_4H_3O) - The highest score in MetFrag
192.9466	$C_6H_4Cl_2O_3$	4.5	0.245	11.1	√	√√	x	√√	 *[5-(chloromethyl)-2-furyl] carbonochloridate* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 192.9464 ($C_6H_3Cl_2O_3$) 156.9698 ($C_6H_2ClO_3$) 128.9750 ($C_5H_2ClO_2$) 93.0347 (C_6H_5O) 65.0030 (C_4HO) - The highest score in MetFrag

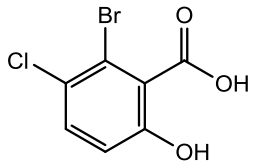
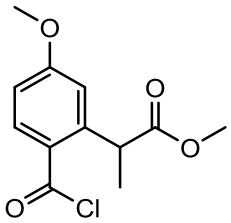
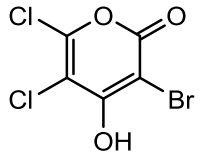
192.9830	$C_7H_8Cl_2O_2$	3.5	0.527	13.1	x	√√	x	x	 *2,2-dichloro-1-(3,4-dihydro-2H-pyran-5-yl)ethanone* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 192.9830 ($C_7H_7Cl_2O_2$) 121.0663 (C_8H_9O) 107.0504 (C_7H_7O) 93.0347 (C_6H_5O) 65.0394 (C_5H_5) - The highest score in MetFrag
204.9465	$C_7H_4Cl_2O_3$	5.5	1.646	20.5	√	x	x	√	 *(2,4-dichloro-6-hydroxy-phenyl) formate* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 204.9468 ($C_7H_3Cl_2O_3$) 160.9571 ($C_6H_3Cl_2O$) 124.9803 (C_6H_2ClO) 113.0251($C_5H_5O_3$) 89.0035 (C_6HO) - The highest score in MetFrag
204.9911	$C_7H_7ClO_5$	4.5	0.467	9.5	x	√√	√	√	 *5-chloro-2-methyl-4-oxo-hex-2-enedioic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 204.9910 ($C_7H_6ClO_5$) 125.0247 ($C_5H_6O_3$) 117.0115 (C_5H_6ClO) 69.0345 (C_4H_5O) - The highest score in MetFrag
204.9911	$C_7H_7ClO_5$	4.5	0.467	10.8	√	√	√	√	 *3-(1-chloropropyl)-2,4-dioxo-oxetane-3-carboxylic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 204.9910 ($C_7H_6ClO_5$) 125.0246 ($C_6H_5O_3$) 169.0144 ($C_7H_5O_5$) 97.0298 ($C_5H_5O_2$) - The highest score in MetFrag

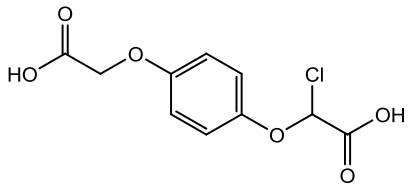
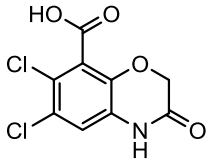
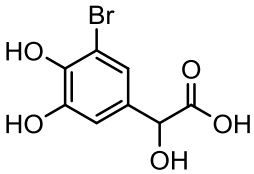
212.8921	$C_5HCl_3O_3$	4.5	2.997	13.5	√√√	√√√	x	√√√	 *3,4,5-trichlorofuran-2-carboxylic acid* (CL 3)	- Isotopic pattern of Cl_3 - Characteristic fragments: 212.8919 ($C_5Cl_3O_3$) 177.9231 ($C_5Cl_2O_3$) 168.9021 (C_4Cl_3O) 149.9282 ($C_4Cl_2O_2$) - The highest score in MetFrag
212.8921	$C_5HCl_3O_3$	4.5	0.468	14.5	T	x	x	√√	n/a (CL 4)	- Isotopic pattern of Cl_3 - No MS2 available
214.8349	$C_2H_2Br_2O_2$	1.5	1.407	9.56	√√√	√√	√√	√√	 *2,2-dibromoacetic acid (*CL 1)	- Isotopic pattern of Br_2 - Characteristic fragments: 170.8453($CHBr_2$) 78.9190) - The highest score in MetFrag - CONFIRMED with analytical standard
215.0117	$C_9H_9ClO_4$	5.5	2.420	5.5	x	√	x	x	 *methyl 4-chloro-3-hydroperoxy -2-methyl-benzoate* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 215.0118 ($C_9H_8ClO_4$) 197.0013 ($C_9H_6ClO_3$) 169.0067 ($C_8H_6ClO_2$) - The highest score in MetFrag
215.0117	$C_9H_9ClO_4$	5.5	3.808	8.8	x	√	x	x	 *3-(3-chloro-4-hydroxy-phenyl)-2-hydroxy-propanoic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 215.0118 ($C_9H_8ClO_4$) 171.0221 ($C_8H_8ClO_2$) 155.9986 ($C_7H_5ClO_2$) 135.0455 ($C_8H_7O_2$) 127.0406 ($C_6H_7O_3$) 91.0192 (C_6H_3O) - The highest score in MetFrag

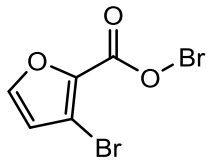
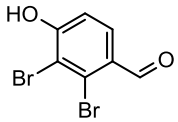
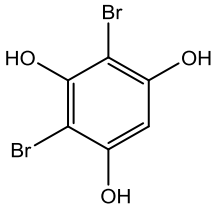
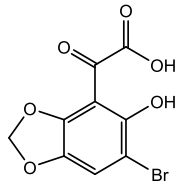
215.0117	$C_9H_9ClO_4$	5.5	1.815	10.1	X	√	X	√	 *2-[2-chloro-4-(hydroxymethyl)phenoxy] acetic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 215.0120 ($C_9H_8ClO_4$) 171.0224 ($C_8H_8ClO_2$) 155.9982 ($C_7H_5ClO_2$) 135.0456 ($C_8H_7O_2$) 107.0506 (C_7H_7O) 91.0193 (C_6H_3O) - The highest score in MetFrag
215.0117	$C_9H_9ClO_4$	5.5	3.342	13.9	x	√√	x	x	 *2-(2-chloro-6-hydroxy-4,5-dihydrocyclopenta[b]furan-6-yl)acetic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 215.0120 ($C_9H_8ClO_4$) 187.9884 ($C_7H_5ClO_4$) 171.0224 ($C_8H_8ClO_2$) 155.9982 ($C_7H_5ClO_2$) 141.9828 ($C_6H_3ClO_2$) 135.0456 ($C_8H_7O_2$) 109.0662 (C_7H_9O) - The highest score in MetFrag
216.9505	$C_7H_7BrO_3$	4.5	-0.230	11.1	√	√√	√	√	 *4-bromo-5-methoxy-benzene-1,3-diol* (CL 3)	- Isotopic pattern of Br - Characteristic fragments: 216.9507 ($C_7H_6BrO_3$) 137.0248 ($C_7H_5O_3$) 117.0115 (C_5H_6ClO) 78.9190 (Br) - The highest score in MetFrag
216.9909	$C_8H_7ClO_5$	5.5	-0.066	10	x	√√	x	√	 *methyl 4-chloro-2,3,5-trihydroxy-benzoate* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 219.9909 ($C_8H_6ClO_5$) 173.0012 ($C_7H_6ClO_3$) 137.246 $C_6H_3ClO_3$) 137.0246 ($C_7H_5O_3$) 109.02976 ($C_6H_5O_2$)

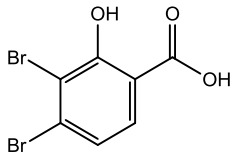
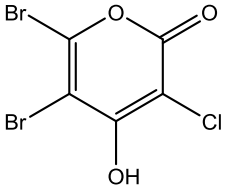
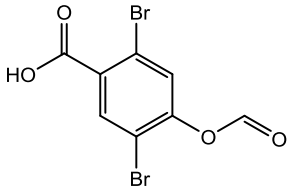
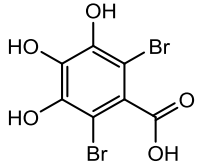
										- The highest score in MetFrag
222.8805	$C_5H_2BrClO_3$	4.5	1.716	10.3/	√√	√√√	√√	√√	 *5-bromofuran-2-yl carbonochloridate* (CL 3)	- Isotopic pattern of BrCl - Characteristic fragments: 222.8803 ($C_5HBrClO_3$) 147.9571 (C_4HClO_4) 143.9622 (C_5HClO_3) 98.9645 (C_4ClO) 78.9190 (Br) - The highest score in MetFrag
		4.5	2.299	11.7	√	X	X	√	n/a (CL 4)	- Isotopic pattern of BrCl - Equal fragmentation pattern than the one eluting at 10.3
228.9232	$C_6H_5Cl_3O_3$	3.5	1.541	11.9	√	√√	X	√√	 *(E)-2-acetyl-4,4,4-trichloro-but-2-enoic acid* (CL 3)	- Isotopic pattern of Cl_3 - Characteristic fragments: 192.9468 ($C_6H_3Cl_2O_3$) 177.9234 ($C_5Cl_2O_3$) 149.9283 ($C_4Cl_2O_2$) 67.0189 (C_4H_3O) - The highest score in MetFrag
228.9465	$C_9H_3Cl_2O_3$	7.5	0.119	19.3	√	√√	√	√	 *3-(2-chloro-2-oxo-acetyl)benzoyl chloride* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 228.9465 ($C_9H_2Cl_2O_3$) 193.9778 ($C_9H_3ClO_3$) 165.9829 ($C_8H_3ClO_2$) - The highest score in MetFrag
231.0066	$C_9H_9ClO_5$	5.5	-0.235	10.2	T	√√	√	T	 *3,4-dihydroxy-5-(2-hydroxyethoxy)benzoyl chloride* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 231.0065 ($C_9H_8ClO_5$) 198.9804 ($C_8H_4ClO_4$) 187.0166 ($C_8H_8ClO_3$) 170.9855 ($C_7H_4ClO_3$) 154.9906 ($C_7H_4ClO_2$)

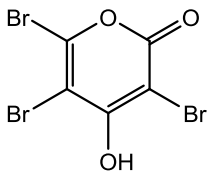
										67.0187 (C_4H_3O) - The highest score in MetFrag
231.0066	$C_9H_9ClO_5$	5.5	0.068	14.0	T	√√	x	x	 *2-(2-chloro-3,4-dihydroxy-6-methyl-phenyl)-2-hydroxy-acetic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 231.0065 ($C_9H_8ClO_5$) 187.0166 ($C_8H_8ClO_3$) 170.9855 ($C_7H_4ClO_3$) 154.9908 ($C_7H_4ClO_2$) 121.0298 ($C_7H_5O_2$) 79.0190 (C_5H_3O) - The highest score in MetFrag
236.8959	$C_6H_4BrClO_3$	4.5	0.939	11.7	√√	√√	√	√√	 *2-bromo-4-chloro-benzen-1,2,5-triol* (CL 3)	- Isotopic pattern of BrCl - Characteristic fragments: 236.8960 ($C_6H_3BrClO_3$) 200.9194 ($C_6H_2BrO_3$) 156.9701 ($C_6H_2ClO_3$) 78.9189 (Br) -The highest score in MetFrag
236.8959	$C_6H_4BrClO_3$	4.5	0.939	11.9	√√	√√	√	√√	 *2-bromo-6(chloromthyl)-3hydroxy-pyran-4-one* (CL 3)	- Isotopic pattern of BrCl - Characteristic fragments: 156.9701 ($C_6H_2ClO_3$) 78.9189 (Br) - The highest score in MetFrag
243.0063	$C_{10}H_9ClO_5$	6.5	-1.047	12.4/ 10.7	x	√√	x	√	n/a (CL 4)	- Isotopic pattern of Cl - No MS2 available
245.0217	$C_{10}H_{11}ClO_5$	5.5	-1.242	12.7	x	√√	x	x	n/a (CL 4)	- Isotopic pattern of Cl - No MS2 available
247.0014	$C_9H_9ClO_6$	5.5	0.409	9.9	x	√√	x	√	n/a (CL 4)	- Isotopic pattern of Cl - No MS2 available

248.8960	$C_7H_4BrClO_3$	5.5	0.211	20.9	√√	x	x	√√	 *2-bromo-3-chloro-6-hydroxy-benzoic acid* (CL 3)	- Isotopic pattern of BrCl - Characteristic fragments: 248.8960 ($C_7H_3BrClO_3$) 204.9062 (C_6H_3BrClO) 168.9298 (C_6H_2BrO) 124.9802 (C_6H_2ClO) 78.9189 (Br) - The highest score in MetFrag
255.0431	$C_{12}H_{13}ClO_4$	6.5	0.471	14.2	x	√√	x	X	 *methyl 2-(2-chlorocarbonyl-5-methoxy-phenyl)propanoate* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 255.0428 ($C_{12}H_{12}ClO_4$) 211.0974 ($C_{11}H_{15}O_4$) 193.08707 ($C_4Cl_2O_4$) 167.1078 ($C_{10}H_{15}O_2$) 149.0971 ($C_{10}Cl_{13}O$) 109.0659 (C_7H_9O) 58.9692 (C_2Cl) 59.0135 ($C_2H_3O_2$) - The highest score in MetFrag
256.8413	$C_5HBrCl_2O_3$	4.5	1.130	13.6	√√√	√√√	X	√√√	 *3-bromo-5,6-dichloro-4-hydroxy-pyran-2-one* (CL 3)	- Isotopic pattern of $BrCl_2$ - Characteristic fragments: 256.8414 ($C_5BrCl_2O_3$) 181.9181 ($C_4Cl_2O_4$) 177.9231 ($C_5Cl_2O_3$) 149.9282 ($C_4Cl_2O_2$) 98.9645 (C_4ClO) 78.9189 (Br) 58.9692 (C_2Cl) - The highest score in MetFrag

259.0015	$C_{10}H_9ClO_6$	6.5	-0.845	9.7/ 9.1	X	√√	X	X	 *2-[4-(carboxymethoxy) phenoxy]-2-chloro-acetic acid* (CL 3)	- Isotopic pattern of Cl - Characteristic fragments: 259.0012 ($C_{10}H_8ClO_6$) 215.0120 ($C_9H_8ClO_4$) 187.9877 ($C_7H_5ClO_4$) 171.0220 ($C_7H_5ClO_2$) 155.9983 ($C_8H_9O_3$) 135.0451 ($C_8H_7O_2$) 107.0505 (C_7H_7O) 93.0348 (C_6H_5O) - The highest score in MetFrag
259.9520	$C_9H_5Cl_2O_4N$	7.5	-2.063	19.5	√√	x	x	√√	 *6,7-dichloro-3-oxo-4H-1,4-benzoxazine-8-carboxylic acid* (CL 3)	- Isotopic pattern of Cl_2 - Characteristic fragments: 259.9517 ($C_9H_4Cl_2O_4N$) 215.9624 ($C_8H_4Cl_2O_2N$) 171.9728 ($C_7H_4Cl_2N$) 135.9961 (C_7H_3ClN) 100.0195 (C_7H_2N) - The highest score in MetFrag
260.9406	$C_8H_7BrO_5$	5.5	-0687	9.88	√	√√	T	x	 *2-(3-bromo-4,5-dihydroxy-phenyl)-2-hydroxy-acetic acid* (CL 3)	- Isotopic pattern of Br - Characteristic fragments: 260.9406 ($C_8H_6BrO_5$) 216.9506 ($C_7H_6BrO_3$) 181.0508 ($C_9H_9O_4$) 109.0297 ($C_6H_5O_2$) 137.0246 ($C_7H_5O_3$) 78.9189 (Br) - The highest score in MetFrag

266.8296	$C_5H_2Br_2O_3$	4.5	-0.646	10.6	√√	√√	T	X	 *bromo-3-bromofuran-2-carboxylate* (CL 3)	- Isotopic pattern of Br_2 - Characteristic fragments: 266.8297 ($C_5HBr_2O_3$) 187.9119 (C_5HBrO_3) 142.9138 (C_4BrO) 78.9190 (Br) - The highest score in MetFrag
276.8505	$C_7H_4Br_2O_2$	5.5	1.669	19.2	√	X	X	X	 *2,3-dibromo-4-hydroxy-benzaldehyde* (CL 3)	- Isotopic pattern of Br_2 - Characteristic fragments: 276.8505 ($C_7H_3Br_2O_2$) 78.9190 (Br) - The highest score in MetFrag
280.8454	$C_6H_4Br_2O_3$	4.5	-0.436	12.5	√√	√√	√	X	 *2,4-dibromobenzene-1,3,5-triol* (CL 3)	- Isotopic pattern of Br_2 - Characteristic fragments: 280.8455 ($C_6H_3Br_2O_3$) 200.9194 ($C_6H_2BrO_3$) 113.0247 ($C_5H_5O_3$) 78.9190 (Br) - The highest score in MetFrag
286.9196	$C_9H_5BrO_6$	7.5	1.486	16.0	√√	x	x	√	 *2-(6-bromo-5-hydroxy-1,3-benzodioxol-4-yl)-2-oxo-acetic acid* (CL 3)	- Isotopic pattern of Br - Characteristic fragments: 242.9305 ($C_8H_4BrO_4$) 214.9351 ($C_7H_4BrO_3$) 170.9453 (C_6H_4BrO) 78.9190 (Br) 65.0032 (C_4HO) - The highest score in MetFrag
286.9520	$C_{11}H_6Cl_2O_5$	8.5	0.063	18.9	x	√√	√	√	n/a (CL 4)	- Isotopic pattern of Cl_2 - No MS2 available

292.8454	$C_7H_4Br_2O_3$	5.5	1.187	21.9	√√	x	x	x	 *3,4-dibromo-2-hydroxy-benzoic acid* (CL 3)	- Isotopic pattern of Br_2 - Characteristic fragments: 292.8454 ($C_7H_3Br_2O_3$) 248.8556 ($C_6H_3Br_2O$) 168.9296 (C_6H_2BrO) 78.9189 (Br) - The highest score in MetFrag
300.7908	$C_5HBr_2ClO_3$	4.5	0.565	14.1	√√√	√√√	x	x	 *3-chloro-5,6-dibromo-4-hydroxy-pyran-2-one* (CL 3)	- Isotopic pattern of Br_2Cl - Characteristic fragments: 300.7909 ($C_5Br_2ClO_3$) 225.8674(C_4BrClO_4) 221.8725(C_5BrClO_3) 193.8773 (C_4BrClO_2) 98.9645 (C_4ClO) 78.9189 (Br)
318.9412	$C_{11}H_6Cl_2O_7$	8.5	2.442	15.0	√√	√√	√	√√	n/a (CL 4)	- Isotopic pattern of Cl_2 - No MS2 available
320.8404	$C_8H_4Br_2O_4$	6.5	0.695	19.0	√√	X	X	X	 *2,5-dibromo-4-formyloxy-benzoic acid* (CL 3)	- Isotopic pattern of Br_2 - Characteristic fragments: 276.85054 ($C_7H_3Br_2O_2$) 248.8555 ($C_6H_3Br_2O$) 168.9295 (C_6H_2BrO) 78.9189 (Br) - The highest score in MetFrag
324.8353	$C_7H_4Br_2O_5$	5.5	-0.190	12.0	√√	√√	T	X	 *2,5-dibromotrihydroxy-benozic acid* (CL 3)	- Isotopic pattern of Br_2 - Characteristic fragments: 244.9086 ($C_7H_2BrO_5$) 200.9194 ($C_6H_2BrO_3$) 78.9189 (Br) - The highest score in MetFrag

344.7403	$C_5HBr_3O_3$	4.5	1.030	13.8	√√√	√√√	X	X	 *3,5,6-tribromo-4-hydroxy-pyran-2-one* (CL 3)	- Isotopic pattern of Br_3 - Characteristic fragments: 344.7405 ($C_5Br_3O_3$) 269.8173 ($C_4Br_2O_4$) 265.8221 ($C_5Br_2O_3$) 237.8271 ($C_4Br_2O_2$) 186.9039 (C_5BrO_3) 142.9141 (C_4BrO) 78.9190 (Br)

*X presence not confirmed, √√√ peak area>$10e^8$, √√ peak area>$10e^7$, √ peak area >$10e^6$, T: Trace amounts.