Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Supplementary Information

Tracking the formation of new brominated disinfection by-products during the seawater desalination process

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Table S1. Filtered water sample characteristics before and after solid phase extraction (SPE). All averages are reported ± standard error (n = 2). Abbreviation definitions are given below the table.

		Before SPE							Post SPE			DOC Eff. (%)
Sample	ID	Salinity	pH	DOC (mg L^{-1})	TDN (mg L^{-1})	SUVA (L mg^{-1} m^{-1})	a(300) (m^{-1})	$S_{300\text{-}500}$ (nm^{-1})	DOC (mg L^{-1})	TDN (mg L^{-1})	OrganoBr (µg L^{-1})	
Raw water	RW	21	7.4	4.3 ± 0.07	0.41 ± 0.06	2.8	12.5	0.019	2.1 ± 0.7	BD	23 ± 6	50 ± 17
Post pretreatment	PT	21	ND	3.9 ± 0.09	0.30 ± 0.06	1.9	6.3	0.024	1.5 ± 0.1	BD	330 ± 40	38 ± 3
Reject (brine) water	BW	60	7.8	10 ± 0.2	0.68 ± 0.06	1.9	17.6	0.024	4.9 ± 1.2	BD	570 ± 40	48 ± 13
RO permeate	ROP	0	ND	BD	BD	BD	0.2	ND	BD	BD	BD	
Drinking water	DW	0	7.5	BD	BD	BD	2.5	ND	BD	BD	7 ± 5	
RW + Cl_2				3.9 ± 0.04	BD	1.8	4.7	0.029	ND	ND	ND	
RW + Cl_2 + $Na_2S_2O_3$	RW + Cl_2			4.1 ± 0.06	BD	1.8	4.8	0.023	ND	ND	310 ± 20	

DOC: dissolved organic carbon
TDN: total dissolved nitrogen
SUVA: specific UV absorbance, or absorbance at 254 nm normalized to pathlength (L, m) and DOC concentration A(254)/(L×DOC)
a(300): the absorption coefficient at 300 nm determined using Equation 1.
$S_{300\text{-}500}$: the spectral slope of ln(a(λ)) versus wavelength, determined between 300 and 500 nm.
OrganoBr: total extractable organic bromine
DOC Eff.: extraction efficiency for DOC using PPL and WAX cartridges, or $100\times(DOC_{post\ SPE}/DOC_{before\ SPE})$
BD: below detection
ND: not determined

Table S2. Intensity-weighted (wt) average (± standard error) molecular characteristics of water samples extracted using a PPL (top) and WAX (bottom) solid phase extraction procedure and analyzed using FT-ICR-MS. These characteristics were determined for assigned molecular compositions containing only carbon, hydrogen, and oxygen (CHO), CHO + nitrogen (CHNO) assignments, CHO + sulfur (CHOS) assignments, CHO + bromine (CHOBr) assignments, CHNO + bromine (CHNOBr) assignments, and CHOS + bromine (CHOSBr) assignments. CHO, CHNO, and CHOS formulas that were found only in raw water PPL extracts (unique RW) and only in reject/brine water PPL extracts (unique BW) are also listed. Abbreviation definitions are given below the table.

PPL extracts	**MW_{wt} (Da)**	**O/C_{wt}**	**H/C_{wt}**	**DBE_{wt}**	**Cos_{wt}**
CHO assignments					
RW (n = 1908)	464.0 ± 89	0.49 ± 0.11	1.16 ± 0.20	10.2 ± 2.4	-0.18 ± 0.34
Unique RW (n = 70)	553.0 ± 89	0.44 ± 0.09	0.83 ± 0.21	17.0 ± 2.4	0.06 ± 0.38
PT (n = 1160)	463.6 ± 94	0.55 ± 0.12	1.13 ± 0.20	10.1 ± 2.6	-0.03 ± 0.36
RW + Cl_2 (n = 1583)	426.4 ± 84	0.50 ± 0.12	1.16 ± 0.19	9.3 ± 2.2	-0.16 ± 0.34
BW (n = 1754)	462.3 ± 82	0.52 ± 0.13	1.17 ± 0.20	9.9 ± 2.1	-0.14 ± 0.37
Unique BW (n = 53)	482.2 ± 145	0.71 ± 0.12	1.25 ± 0.23	8.5 ± 3.1	0.18 ± 0.33
CHNO assignments					
RW (n = 1293)	471.2 ± 75	0.47 ± 0.09	1.13 ± 0.18	10.1 ± 2.4	0.05 ± 0.28
Unique RW (n = 114)	450.0 ± 66	0.44 ± 0.08	0.94 ± 0.18	13.2 ± 2.0	0.22 ± 0.31
PT (n = 723)	428.8 ± 81	0.53 ± 0.09	1.12 ± 0.18	10.1 ± 2.5	0.16 ± 0.29
RW + Cl_2 (n = 1197)	383.0 ± 68	0.48 ± 0.09	1.20 ± 0.18	8.7 ± 2.2	0.01 ± 0.30
BW (n = 1439)	422.1 ± 68	0.50 ± 0.10	1.15 ± 0.20	9.8 ± 2.2	0.07 ± 0.34
BW unique (n = 252)	473.7 ± 113	0.55 ± 0.12	1.16 ± 0.19	10.5 ± 3.0	0.21 ± 0.36
ROP (n = 31)	329.8 ± 66	0.40 ± 0.13	1.42 ± 0.35	6.5 ± 3.3	-0.38 ± 0.49
DW (n = 37)	338.7 ± 58	0.42 ± 0.15	1.55 ± 0.26	5.2 ± 2.6	-0.51 ± 0.43
CHOS assignments					
RW (n = 400)	392.1 ± 59	0.49 ± 0.11	1.27 ± 0.24	7.3 ± 2.3	-0.17 ± 0.40
RW unique (n = 17)	426.1 ± 48	0.39 ± 0.09	1.18 ± 0.42	9.3 ± 4.1	-0.29 ± 0.53
PT n = (557)	423.0 ± 66	0.54 ± 0.11	1.29 ± 0.22	7.4 ± 2.2	-0.09 ± 0.37
RW + Cl_2 (n = 328)	370.9 ± 58	0.47 ± 0.14	1.39 ± 0.25	5.9 ± 2.2	-0.32 ± 0.47
BW (n = 562)	409.3 ± 51	0.53 ± 0.15	1.30 ± 0.22	7.1 ± 1.8	-0.11 ± 0.48
BW unique (n = 177)	468.6 ± 62	0.58 ± 0.10	1.33 ± 0.19	7.6 ± 2.4	-0.06 ± 0.33
ROP (n = 90)	354.6 ± 27	0.28 ± 0.07	1.54 ± 0.14	4.0 ± 1.0	-0.91 ± 0.27
DW (n = 62)	360.4 ± 45	0.39 ± 0.12	1.17 ± 0.39	5.0 ± 1.8	-0.24 ± 0.45
CHOBr assignments					

RW (n = 4)	481.7 ± 100	0.16 ± 0.06	1.21 ± 0.48	10.1 ± 6.1	-0.85 ± 0.45
PT (n = 384)	447.8 ± 86	0.54 ± 0.10	1.10 ± 0.40	8.1 ± 5.2	0.04 ± 0.43
RW + Cl_2 (n = 379)	476.1 ± 81	0.48 ± 0.09	1.19 ± 0.32	7.1 ± 4.0	-0.16 ± 0.38
BW (n = 392)	450.6 ± 55	0.53 ± 0.11	1.12 ± 0.19	8.1 ± 1.9	-0.01 ± 0.34
CHNOBr assignments					
RW (n = 1)	398.0	0.40	1.00	8	0.46
PT (n = 1)	373.0	0.54	0.92	9	0.27
RW + Cl_2 (n = 31)	398.1 ± 31	0.44 ± 0.10	1.05 ± 0.12	8.5 ± 1.9	0.21 ± 0.15
BW (n = 10)	404.7 ± 58	0.47 ± 0.11	1.03 ± 0.11	8.6 ± 2.3	0.34 ± 0.16
CHOSBr assignments					
RW (n = 0)	-	-	-	-	-
PT (n = 108)	448.5 ± 59	0.41 ± 0.08	1.22 ± 0.18	7.2 ± 2.1	-0.21 ± 0.31
RW + Cl_2 (n = 80)	429.9 ± 42	0.38 ± 0.08	1.29 ± 0.17	6.2 ± 1.6	-0.34 ± 0.30
BW (n = 107)	453.8 ± 58	0.39 ± 0.07	1.23 ± 0.18	7.2 ± 2.1	-0.26 ± 0.30
WAX extracts	**MW_{wt} (Da)**	**O/C_{wt}**	**H/C_{wt}**	**DBE_{wt}**	**Cos_{wt}**
CHO assignments					
RW (n = 333)	399.1 ± 72	0.74 ± 0.10	0.94 ± 0.18	9.6 ± 2.4	0.54 ± 0.31
PT (n = 263)	374.0 ± 77	0.77 ± 0.13	0.92 ± 0.21	9.0 ± 2.2	0.63 ± 0.40
RW + Cl_2 (n = 135)	364.8 ± 69	0.77 ± 0.10	0.94 ± 0.21	8.6 ± 1.9	0.60 ± 0.34
BW (n = 428)	378.6 ± 75	0.73 ± 0.12	0.97 ± 0.22	8.9 ± 2.4	0.49 ± 0.37
CHNO assignments					
RW (n = 266)	373.6 ± 62	0.66 ± 0.09	0.94 ± 0.16	9.6 ± 1.9	0.61 ± 0.22
PT (n = 348)	362.6 ± 64	0.68 ± 0.09	0.99 ± 0.19	9.0 ± 2.0	0.60 ± 0.24
RW + Cl_2 (n = 75)	354.0 ± 52	0.72 ± 0.07	0.99 ± 0.16	8.5 ± 1.5	0.67 ± 0.20
BW (n = 378)	363.4 ± 63	0.66 ± 0.09	1.01 ± 0.20	8.9 ± 2.1	0.57 ± 0.25
CHOS assignments					
RW (n = 73)	352.3 ± 117	0.80 ± 0.37	0.72 ± 0.16	7.5 ± 2.4	1.36 ± 0.69
PT (n = 60)	327.2 ± 119	0.89 ± 0.45	0.62 ± 0.19	7.6 ± 3.2	1.65 ± 0.80
RW + Cl_2 (n = 21)	284.6 ± 110	0.77 ± 0.45	0.44 ± 0.16	7.1 ± 2.3	1.85 ± 0.66
BW (n = 128)	330.7 ± 104	0.80 ± 0.34	0.78 ± 0.20	7.1 ± 2.2	1.29 ± 0.68

MW_{wt}: center of mass/molecular weight
O/C: oxygen to carbon ratio
H/C: hydrogen to carbon ratio.
DBE: double bond equivalent
Cos: average carbon oxidation state

Table S3. Br-containing formula assignments found in BW WAX extracts.

Observed ionic mass (*m/z*)	Calculated Mass	Assigned Molecular Formula	Potential structure
214.83479	215.842152	$C_2H_2O_2Br_2$	Dibromoacetic acid
268.84545	269.852717	$C_5H_4O_3Br_2$	3,5-dibromo-4-hydroxypenta-2,4-dienoic acid
300.83527	301.842547	$C_5H_4O_5Br_2$	3,4-dibromo-4-hydroxypent-2-enedioic acid
234.92473	235.932036	$C_6H_5O_5Br$	6-bromobenzene-1,2,3,4,5-pentol
248.94039	249.947686	$C_7H_7O_5Br$	
264.93533	265.942601	$C_7H_7O_6Br$	
276.89896	277.906216	$C_7H_3O_7Br$	
278.950925	279.958251	$C_8H_9O_6Br$	
292.93021	293.937516	$C_8H_7O_7Br$	
306.9095	307.916781	$C_8H_5O_8Br$	
306.9458825	307.953166	$C_9H_9O_7Br$	
334.9408367	335.948081	$C_{10}H_9O_8Br$	
376.9514167	377.958646	$C_{12}H_{11}O_9Br$	
430.96184	431.969211	$C_{15}H_{13}O_{10}Br$	
238.84609	239.853385	$C_3H_2N_2OBr_2$	dibromo-imidazole
249.85084	250.858136	$C_5H_3NOBr_2$	dibromo-pyridone
293.8407	294.847966	$C_6H_3NO_3Br_2$	4,6-dibromo-5-hydroxypicolinic acid
275.91494	276.9222	$C_7H_4NO_6Br$	
250.80184	251.8091377	$CH_2Br_2SO_3$	dibromomethanesulfonic acid
320.80731	321.8146177	$C_4H_4SO_5Br_2$	

Table S4. Summary of water quality parameters for brine water (BW) mysid toxicity test across all treatments.

Water		Temperature (℃)	Salinity (‰)	Dissolved Oxygen (mg L^{-1})	pH
New	Min - Max	25.6 - 26.9	22.26 - 22.90	6.29 - 6.98	8.27 - 8.70
	Average (SD)	26.3 (0.29)	22.54 (0.17)	6.66 (0.13)	8.51 (0.10)
Aged	Min - Max	24.5 - 26.9	22.00 - 24.17	3.89 - 5.92	8.16 - 8.47
	Average (SD)	26.0 (0.59)	22.89 (0.32)	4.81 (0.53)	8.31 (0.07)
Overall[a]	Average (SD)	26.1 (0.54)	22.79 (0.32)	5.36 (0.97)	8.37 (0.12)

[a]Minimum and maximum values are not explicitly included as they are easily derived from new and aged solution ranges. SD = standard deviation.

Table S5. Summary of water quality parameters for receiving water (RW) mysid toxicity test across all treatments.

Water		Temperature (℃)	Salinity (‰)	Dissolved Oxygen (mg L^{-1})	pH
New	Min - Max	24.2 - 26.9	22.40 - 23.21	6.20 - 8.24	8.27 - 8.66
	Average (SD)	26.0 (0.56)	22.75 (0.22)	6.86 (0.33)	8.47 (0.09)
Aged	Min - Max	24.8 - 27.0	22.13 - 24.15	3.60 - 6.81	8.06 - 8.65
	Average (SD)	26.0 (0.51)	23.08 (0.37)	4.86 (0.52)	8.29 (0.08)
Overall [a]	Average (SD)	26.0 (0.53)	22.98 (0.36)	5.47 (1.04)	8.35 (0.11)

[a]Minimum and maximum values are not explicitly included as they are easily derived from new and aged solution ranges. SD = standard deviation.

Table S6. Summary of toxicity endpoints for receiving water (RW) and brine water (BW) mysid toxicity tests.

Water	Endpoint	% Starting Concentration LC_{50} or			% BW or RW		
		NOEC	EC_{50}	IC_{25}	NOEC	LC_{50}	IC_{25}
RW	Mortality	>100	>100	>100	>100	>100	>100
	Growth	>100	>100	>100	>100	NA	>100
BW	Mortality	>100	>100	>100	>36.5	>36.5	>36.5
	Growth	>100	>100	>100	>36.5	NA	>36.5

LC50 calculated for mortality endpoint and EC50 for growth endpoint

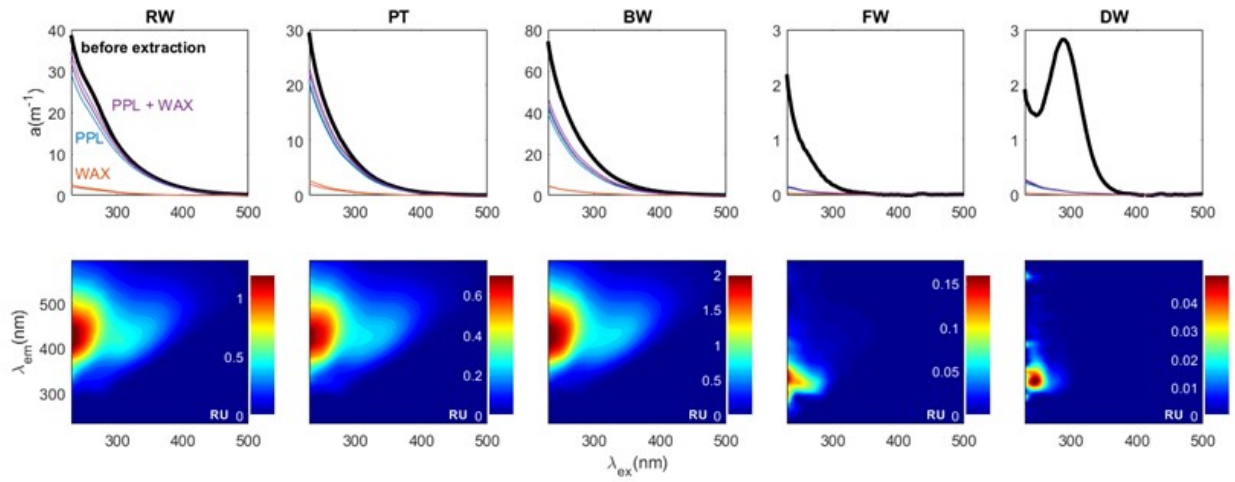

Figure S1. **(top)** Absorption spectra (a(m^{-1})) for raw water (RW), post pretreatment water (PT), RO reject/brine water (BW), RO permeate (ROP), and chlorinated drinking water (DW). Note the difference in scale between samples. Black lines are samples prior to extraction, blue lines are a(m^{-1}) spectra of PPL SPE-DOM samples, red lines are a(m^{-1}) spectra of weak anion exchange (WAX) SPE-DOM samples and purple lines are the sum of PPL and WAX a(m^{-1}) spectra. (**bottom**) Excitation-emission matrix spectra (EEMS) corresponding to water sample a(m^{-1}) spectra (black lines) above. Note the difference in scale between samples SPE-DOM EEMS shown in Figures S2 and S3.

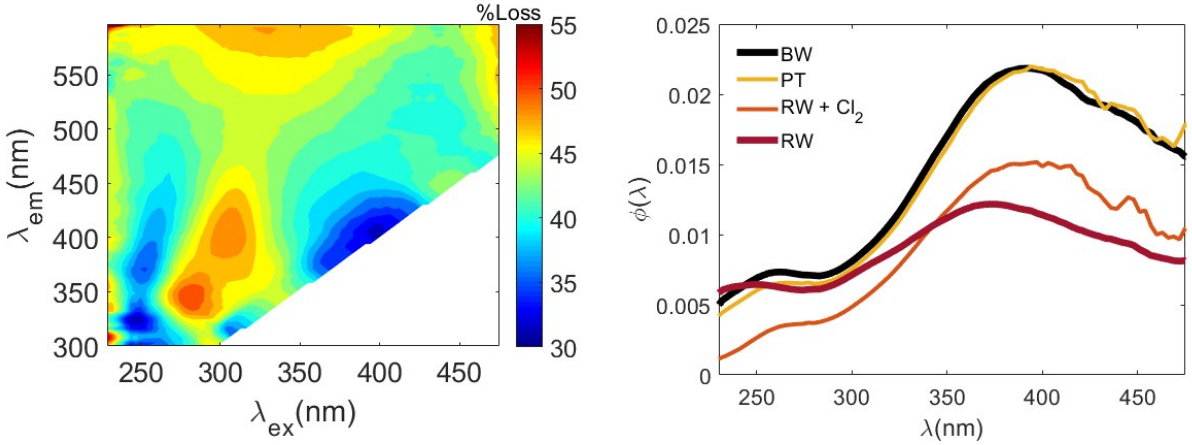

Figure S2. (**left**) Percent fluorescence loss between RW and PT samples. (**right**) Fluorescence apparent quantum yield spectra ($\varphi(\lambda)$) for RW (maroon line), PT (yellow line), RW + Cl_2 (orange line) and BW (black line) samples.

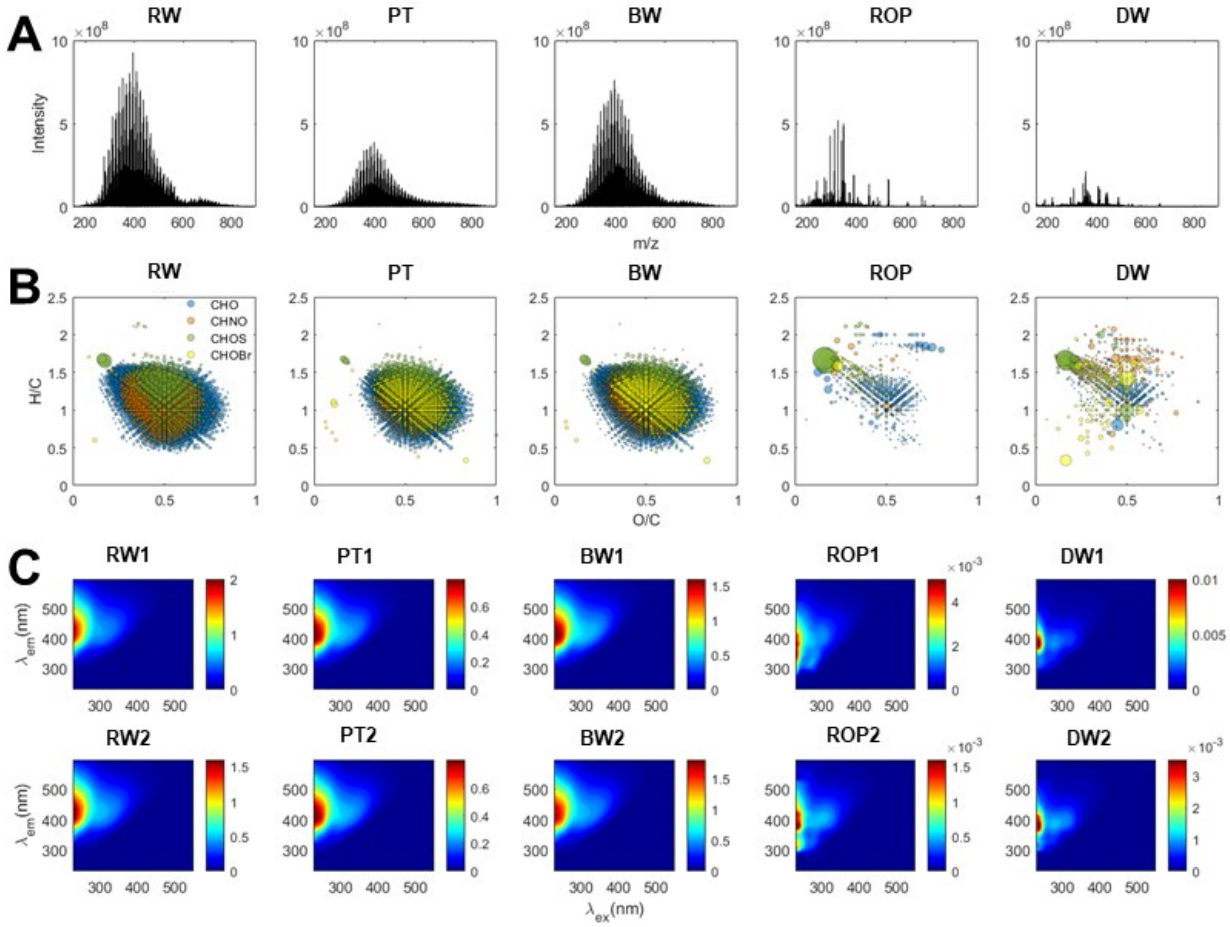

Figure S3. (**A**) FT-ICR-MS mass spectra of PPL extracts for various sample types (RW, PT, BW, ROP and DW) and (**B**) corresponding Van Krevelen diagrams (hydrogen to carbon ratio, H/C versus oxygen to carbon ratio, O/C) of assigned molecular formulas from (**A**). Blue dots are formulas containing only carbon, hydrogen and oxygen (CHO), orange dots are formulas containing CHO + nitrogen (CHNO), green dots are formulas containing CHO + sulfur (CHOS) and yellow dots are formulas containing CHO + bromine (CHOBr). (**C**) EEM spectra of SPE-DOM samples for PPL extracts (note the difference in scale between samples are replicates), highlighting that this SPE technique captures the majority of the features in EEM spectra prior to extraction (Figure 1).

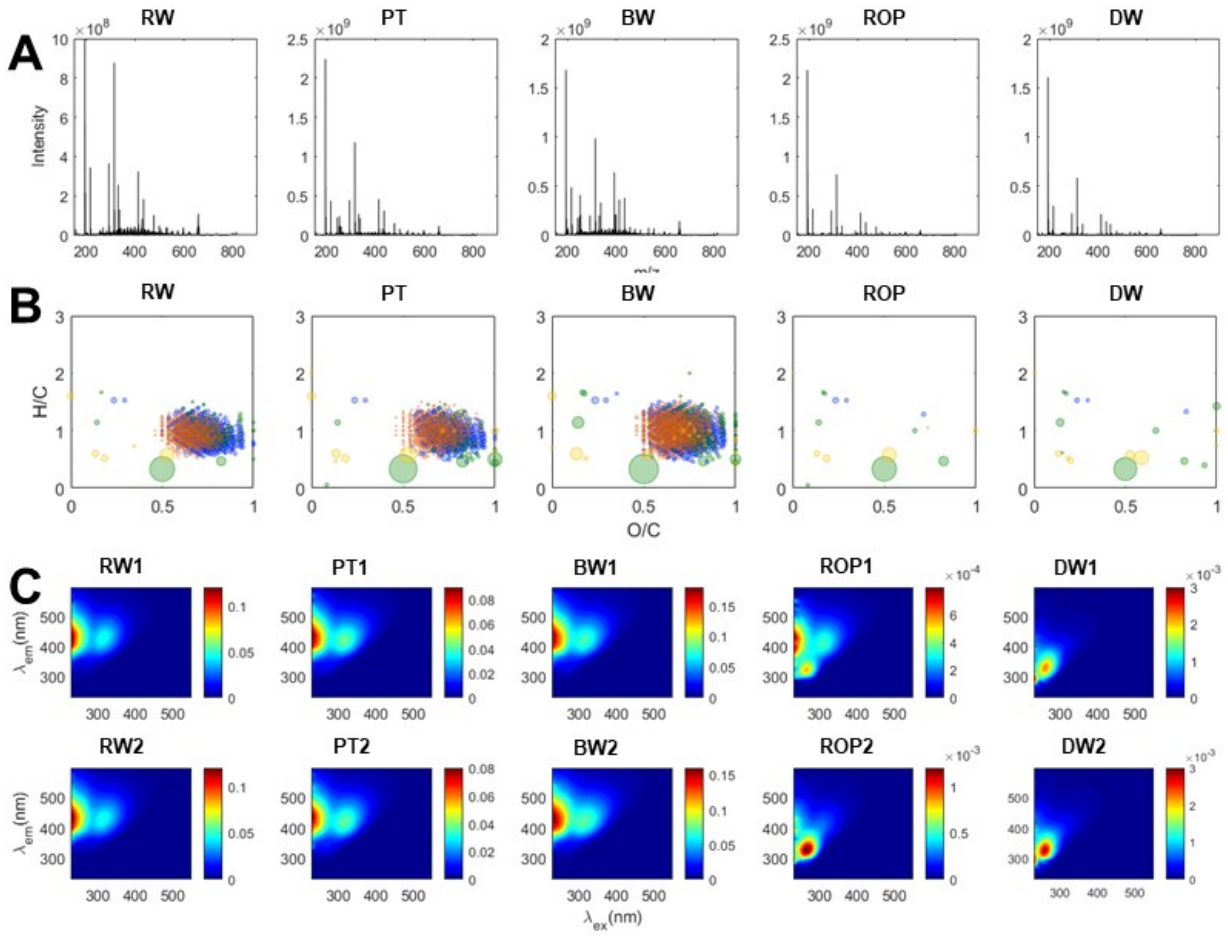

Figure S4. (A) FT-ICR-MS mass spectra of WAX extracts for various sample types (RW, PT, BW, ROP and DW) and (**B**) corresponding Van Krevelen diagrams (hydrogen to carbon ratio, H/C versus oxygen to carbon ratio, O/C) of assigned molecular formulas from (**A**). Blue dots are formulas containing only carbon, hydrogen and oxygen (CHO), orange dots are formulas containing CHO + nitrogen (CHNO), green dots are formulas containing CHO + sulfur (CHOS) and yellow dots are formulas containing CHO + bromine (CHOBr). (**C**) EEM spectra of SPE-DOM samples for WAX extracts (note the difference in scale between samples are replicates. While PPL does capture the majority of fluorescence features observed in water samples prior to extraction, (**C**) highlights additional fluorescence information that is gained from the WAX SPE-DOM samples.

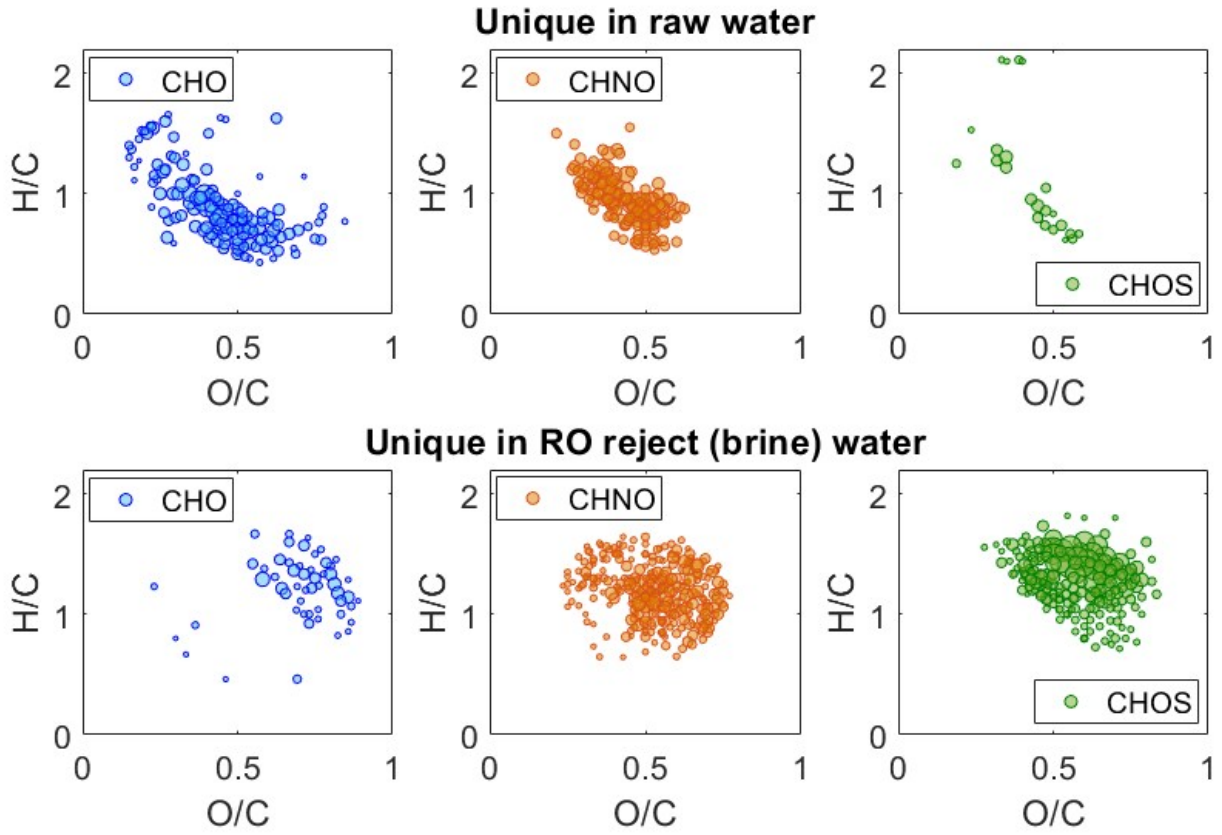

Figure S5. CHO (left, blue circles), CHNO (center, orange circles), and CHOS (right, green circles) that are unique in raw water PPL extracts (top) and those that are unique in reject (brine) water PPL extracts (bottom). Bubble size corresponds to molecular ion intensity.

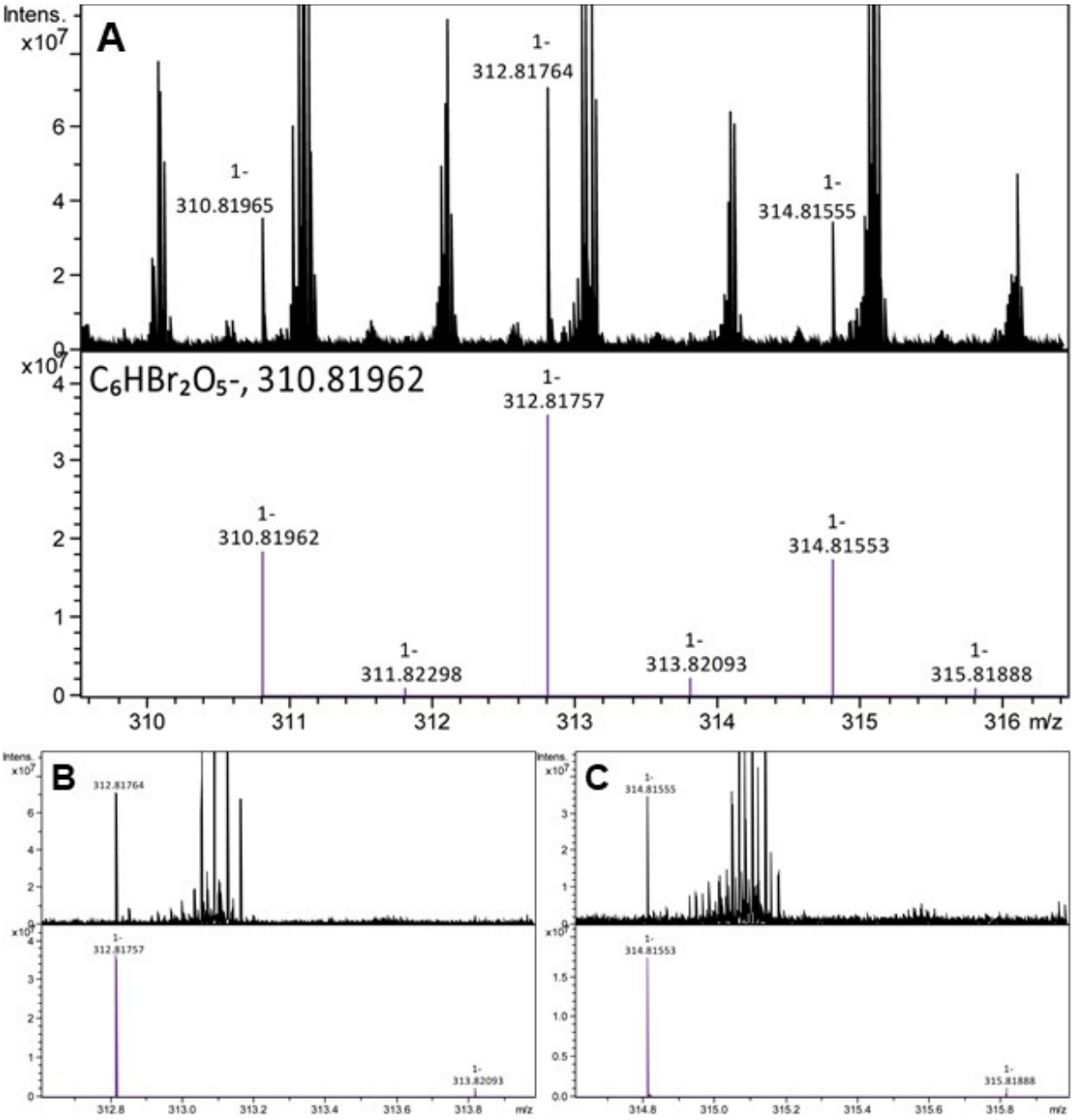

Figure S6. (**A**) Example of the isotope simulation of a brominated molecular ion ($C_6HBr_2O_5^-$, purple ions, bottom) in the reject (brine) water PPL extract (black ions, top) to confirm molecular formula assignments containing bromine. (**B**) and (**C**) are the same as (**A**), but show details of the $C_6H^{79}Br^{81}BrO_5^-$ isotope (**B**) and the $C_6H^{81}Br_2O_5^-$ isotope (**C**). This molecular ion in the PPL extract was further tested by Orbitrap MS/MS, whose result is in listed in Tables 2. Measured and predicted ionic masses and error are given below.

$(M-H)^-$	Measured *m/z*	Predicted *m/z*	Error (ppm)
$C_6H^{79}Br_2O_5^-$	310.81965	310.81962	0.097
$C_6H^{79}Br^{81}BrO_5^-$	312.81764	312.81757	0.224
$C_6H^{81}Br_2O_5^-$	314.81555	314.81553	0.064

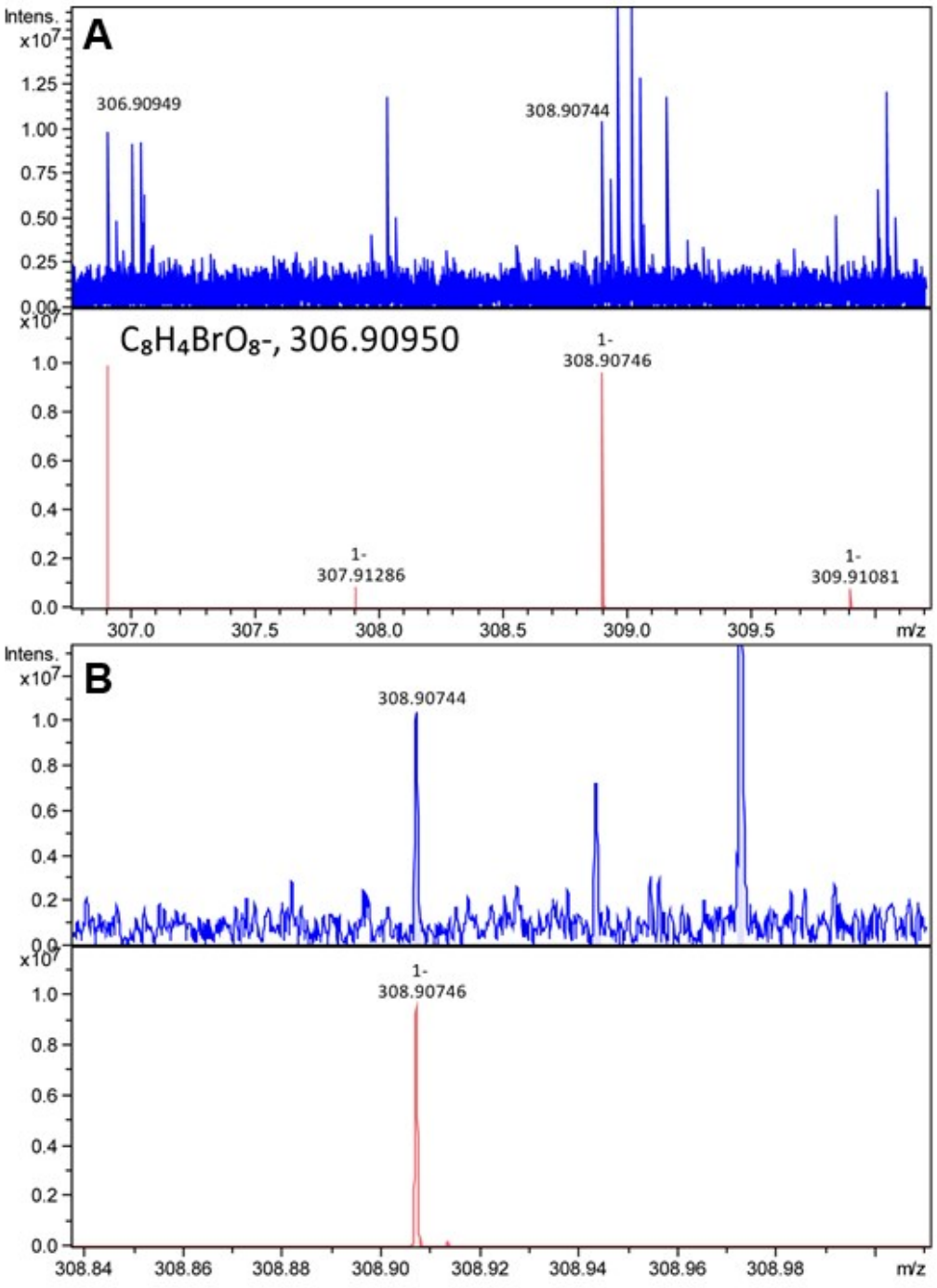

Figure S7. (**A**) Example of the isotope simulation of a brominated molecular ion ($C_8H_4BrO_8^-$, red ions, bottom) in the reject (brine) water WAX extract (blue ions, top) to confirm molecular formula assignments containing bromine. (**B**) shows the details of the $C_8H_4{}^{81}BrO_8^-$ isotope. Measured and predicted ionic masses and error are given below.

$(M-H)^-$	Measured *m/z*	Predicted *m/z*	Error (ppm)
$C_8H_4{}^{79}BrO_8^-$	306.90949	306.9095	0.033
$C_8H_4{}^{81}BrO_8^-$	308.90744	308.90746	0.065

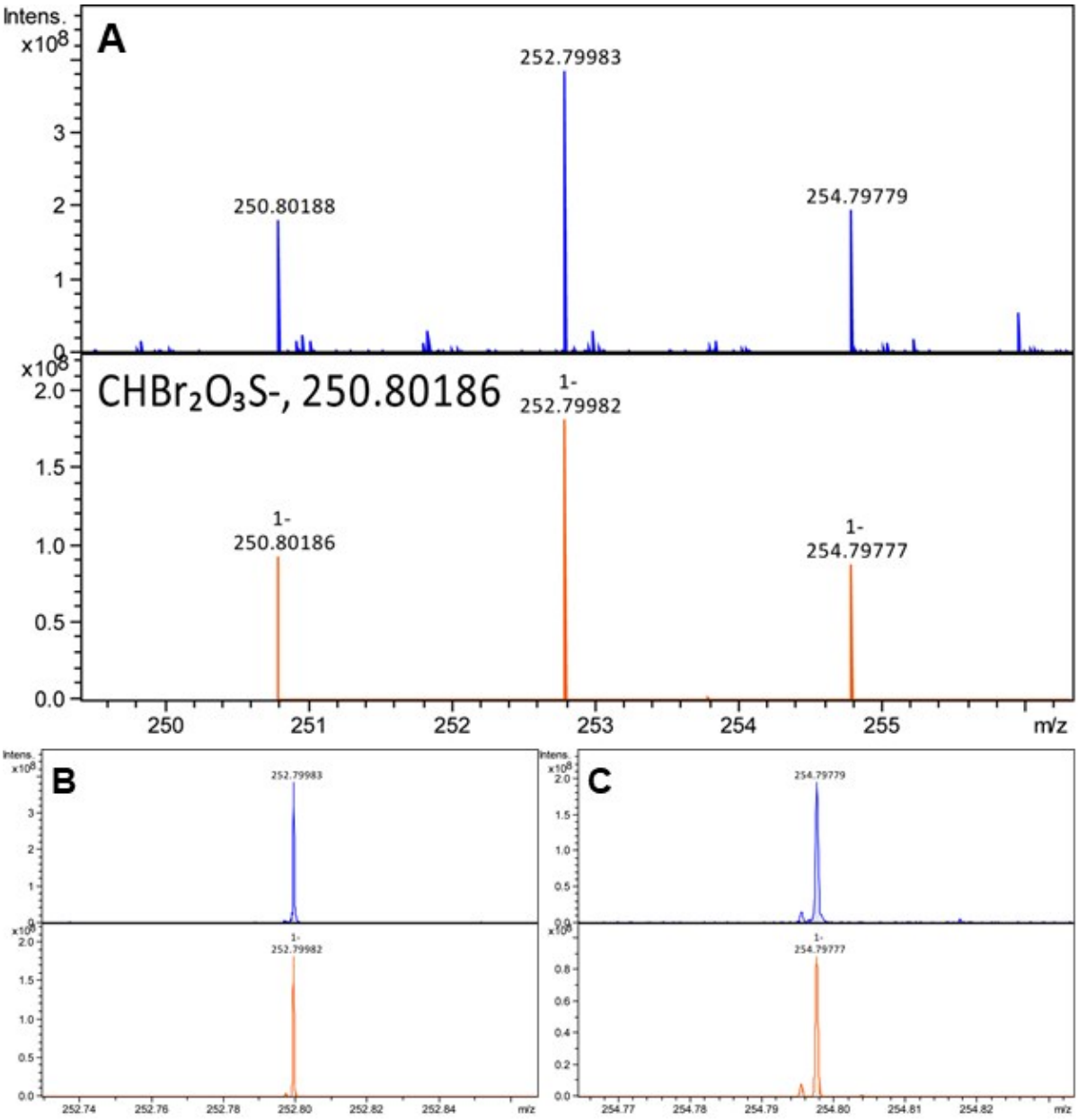

Figure S8. (**A**) Example of the isotope simulation of a molecular ion containing bromine and sulfur ($CHBr_2SO_3^-$, orange ions, bottom) in the reject (brine) water WAX extract (blue ions, top) to confirm molecular formula assignments containing bromine. (**B**) and (**C**) are the same as (**A**), but show details of the $CH^{79}Br^{81}BrSO_3^-$ isotope (**B**) and the $CH^{81}Br_2SO_3^-$ isotope (**C**). This molecular ion in the WAX extract was further tested by Orbitrap MS/MS, whose result is in listed in Tables 3. Measured and predicted ionic masses and error are given below.

$(M-H)^-$	Measured *m/z*	Predicted *m/z*	Error (ppm)
$CH^{79}Br_2SO_3^-$	250.80188	250.80186	0.080
$CH^{79}Br^{81}BrSO_3^-$	252.79983	252.79982	0.040
$CH^{81}Br_2SO_3^-$	254.79779	254.79777	0.079

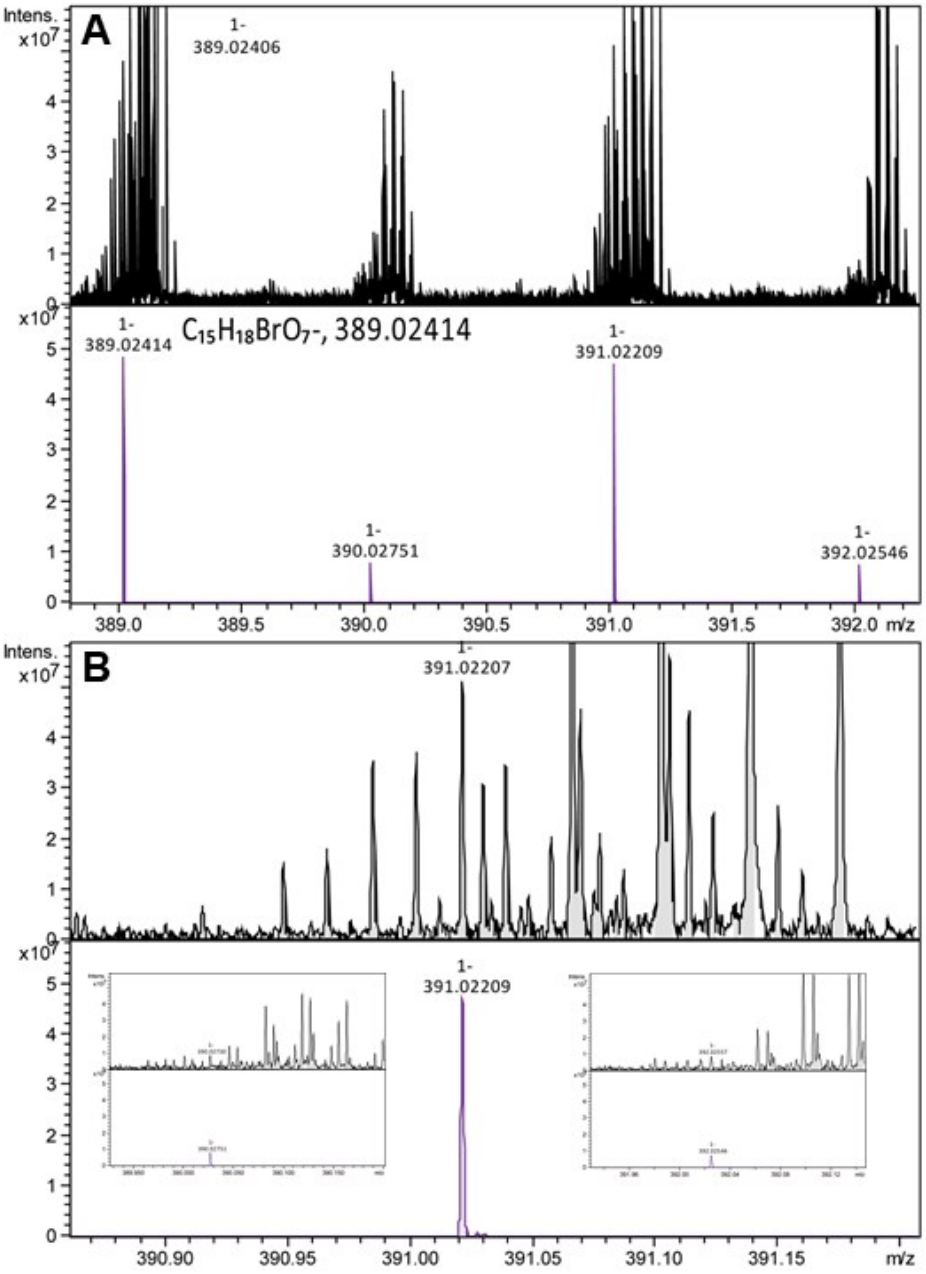

Figure S9. (**A**) Example of the isotope simulation of a brominated molecular ion ($C_{15}H_{18}BrO_7^-$, purple ions, bottom) in the reject (brine) water PPL extract (black ions, top). This simulation is used to confirm this molecular formula assignments containing bromine and without a negative mass defects (e.g. more saturated formulas). (**B**) shows the details of the $C_{15}H_{18}{}^{81}Br\,O_7^-$ isotope and insets in (**B**) show the ^{13}C isotopes. Measured and predicted ionic masses and error are given below.

$(M-H)^-$	Measured *m/z*	Predicted *m/z*	Error (ppm)
$C_{15}H_{18}{}^{79}BrO_7^-$	389.02406	389.02414	0.206
$C_{15}H_{18}{}^{81}Br\,O_7^-$	391.02207	391.02209	0.051

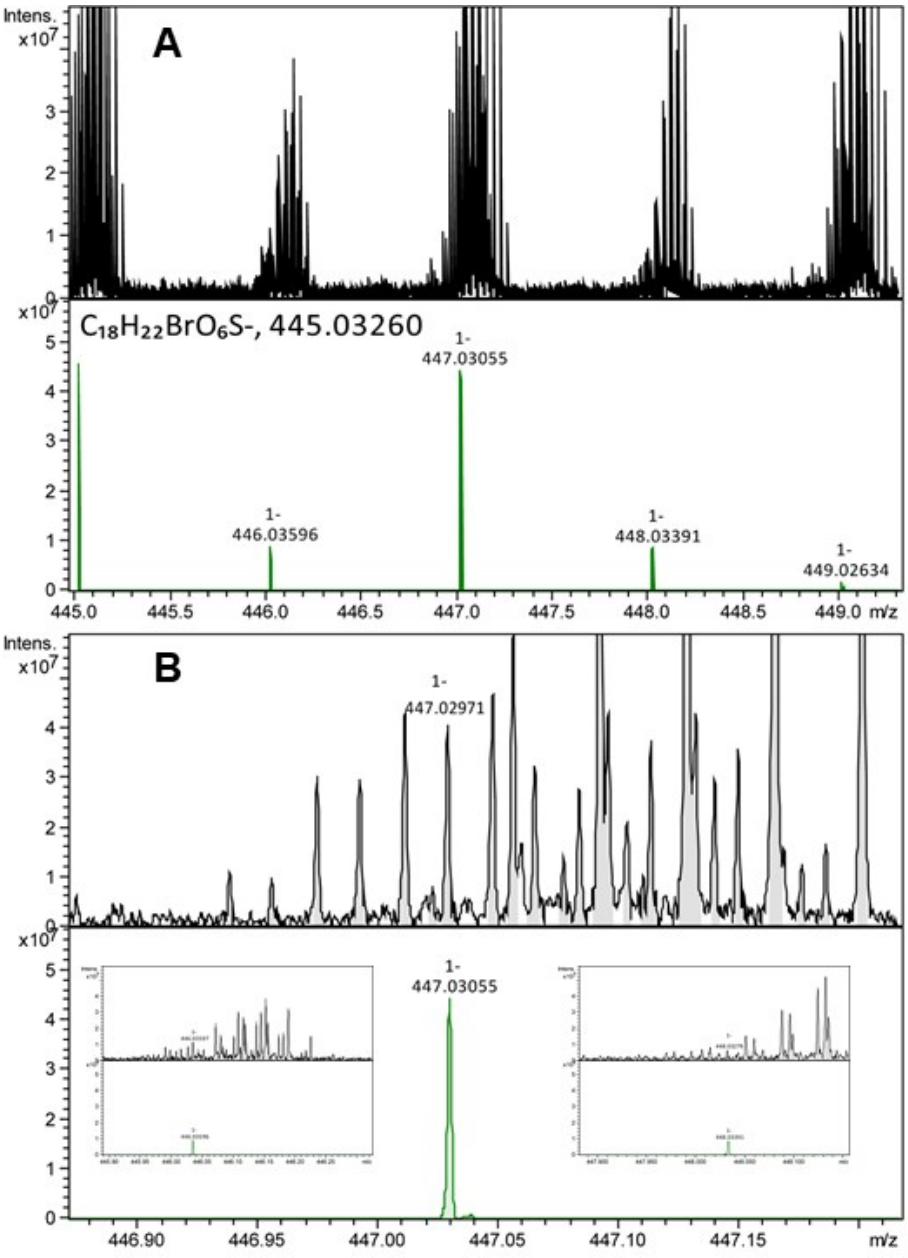

Figure S10. (**A**) Example of the isotope simulation of a molecular ion containing bromine and sulfur ($C_{18}H_{22}BrSO_6^-$, green ions, bottom) in the reject (brine) water PPL extract (black ions, top). This simulation is used to confirm this molecular formula assignments containing bromine and without a negative mass defects (e.g. more saturated formulas). (**B**) shows the details of the $C_{18}H_{22}{}^{81}BrSO_6^-$ isotope and insets in (**B**) show the ^{13}C isotopes. Measured and predicted ionic masses and error are given below.

$(M-H)^-$	Measured *m/z*	Predicted *m/z*	Error (ppm)
$C_{18}H_{22}{}^{79}BrSO_6^-$	445.0327	445.03260	0.165
$C_{18}H_{22}{}^{81}BrSO_6^-$	447.0297	447.03055	1.88

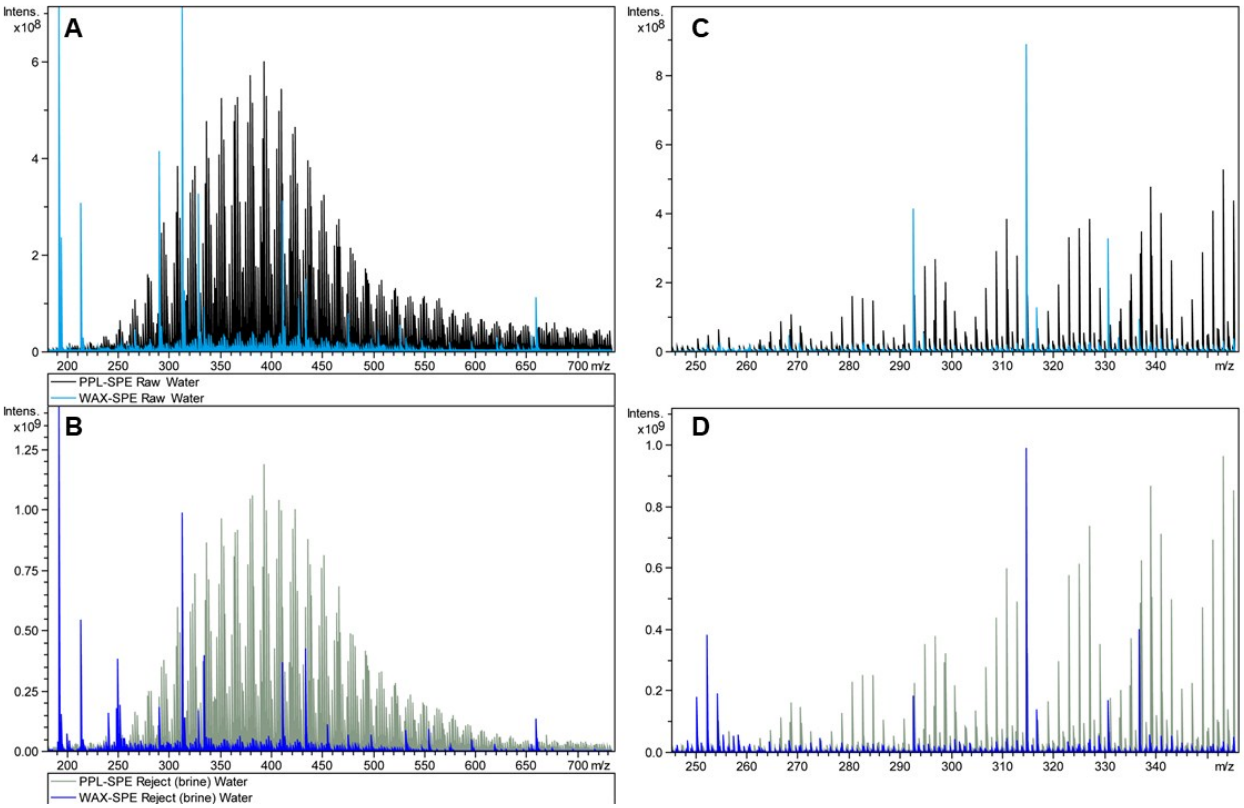

Figure S11. (**A**) FT-ICR mass spectra of raw water extracted by PPL-SPE (black ions) followed by WAX-SPE (light blue ions) and (**B**) FT-ICR mass spectra of RO reject (brine) water extracted by PPL-SPE (gray ions) followed by WAX-SPE (blue ions). (**C**) and (**D**) are FT-ICR mass spectra plotted from 250 to 350 *m/z* for raw water and reject water, respectively. Same colors as (**A**) and (**B**) apply.

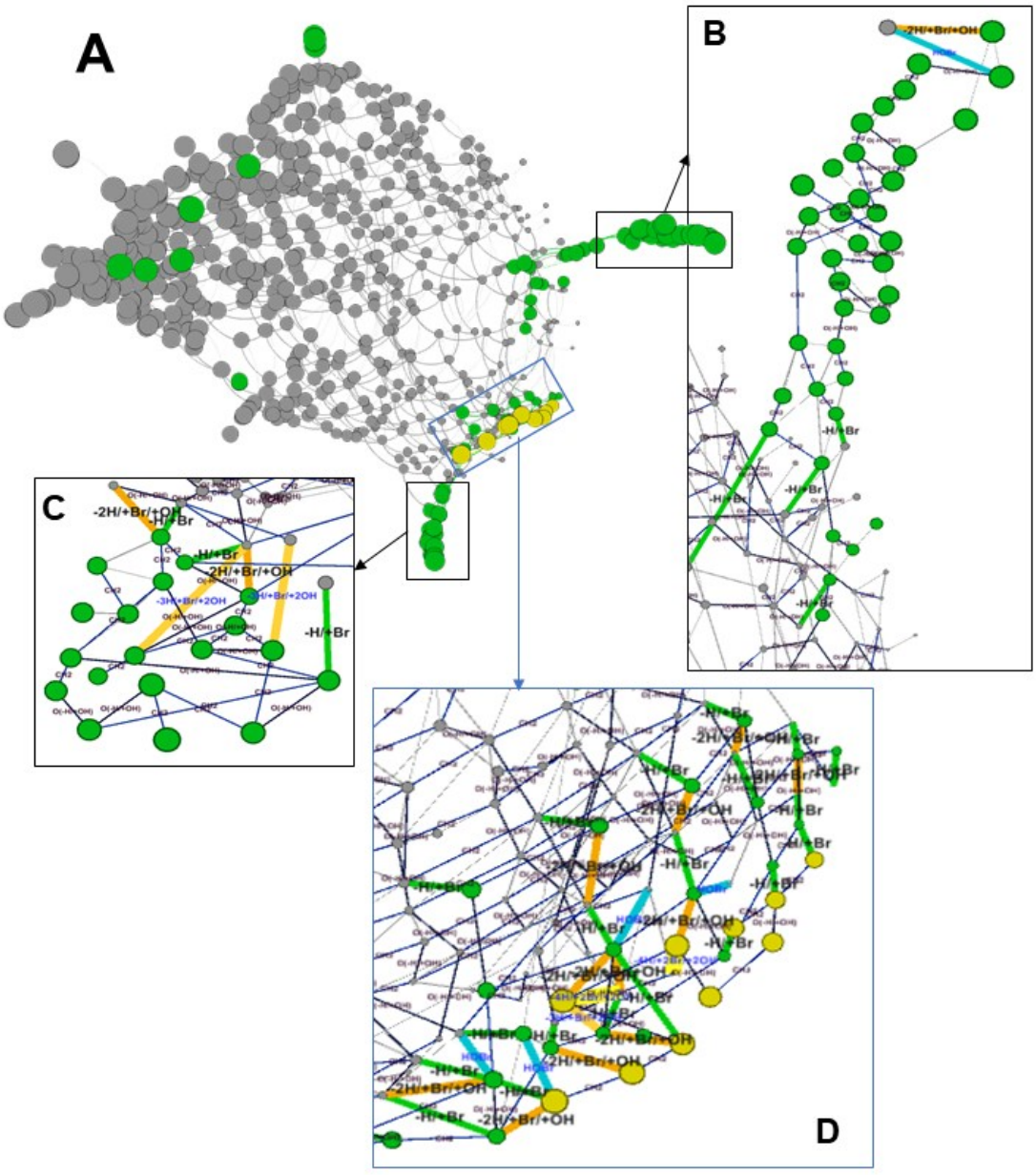

Figure S12. (**A**) Mass difference network analysis of all CHOS (gray circles) in RW, PT, and BW PPL extracts and CHOSBr (green circles) and $CHOSBr_2$ (yellow circles) in PT and BW PPL extracts to see if substitution reactions (-H/+Br, greeen lines), substitution + hydroxylation (e.g. –2H/+Br/+OH, orange and yellow lines) or addition reactions (HOBr, blue lines lines) might explain the formation of Br-DBPs in PT and BW samples. Bubble size corresponds to *m/z* value. (**B** and **C**) highlight pools of CHOSBr formulas that could not be explained by substitution or addition reactions since there are only a few transitions between CHOS and CHOSBr. (**D**) highlights a pool with many –H/+Br transitions and these formulas are in line with the bromination of suspected surfactant metabolites (sulfophenyl carboxylic acids, SPCs). The pool in (**D**) was further tested by mass difference network analysis and those results are shown in Figure 4 and in Figure S13.

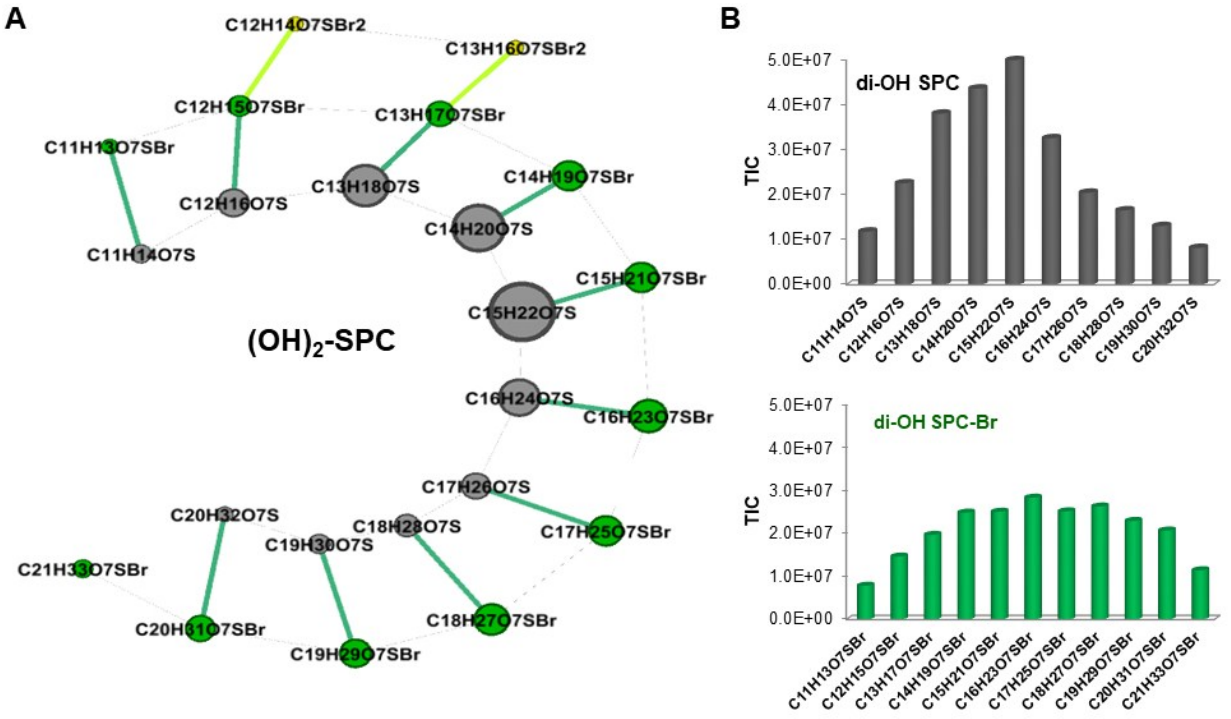

Figure S13. (**A**) Mass difference network analysis of CHOS formulas that match formulas for sulfophenyl carboxylic acids (SPCs) with 2 hydroxylations (+2OH) on the aromatic ring (gray circles) in RW, PT, and BW PPL extracts and CHOSBr formulas (green circles) in PT and BW PPL extracts to see if substitution reactions (H for Br, green lines) might explain the formation of Br-DBPs in PT and BW samples. Yellow lines are also a transition of –H/+Br to $CHOSBr_2$ (yellow circles) molecular formulas (**B**) Total ion count (TIC) versus homologous series (formulas spaced by CH_2) of CHOS formulas (gray, top) and CHOSBr formulas (green, bottom) in the network displayed in (**A**).