

Electronic Supplementary Information

Waterworks-specific composition of drinking water disinfection by-products

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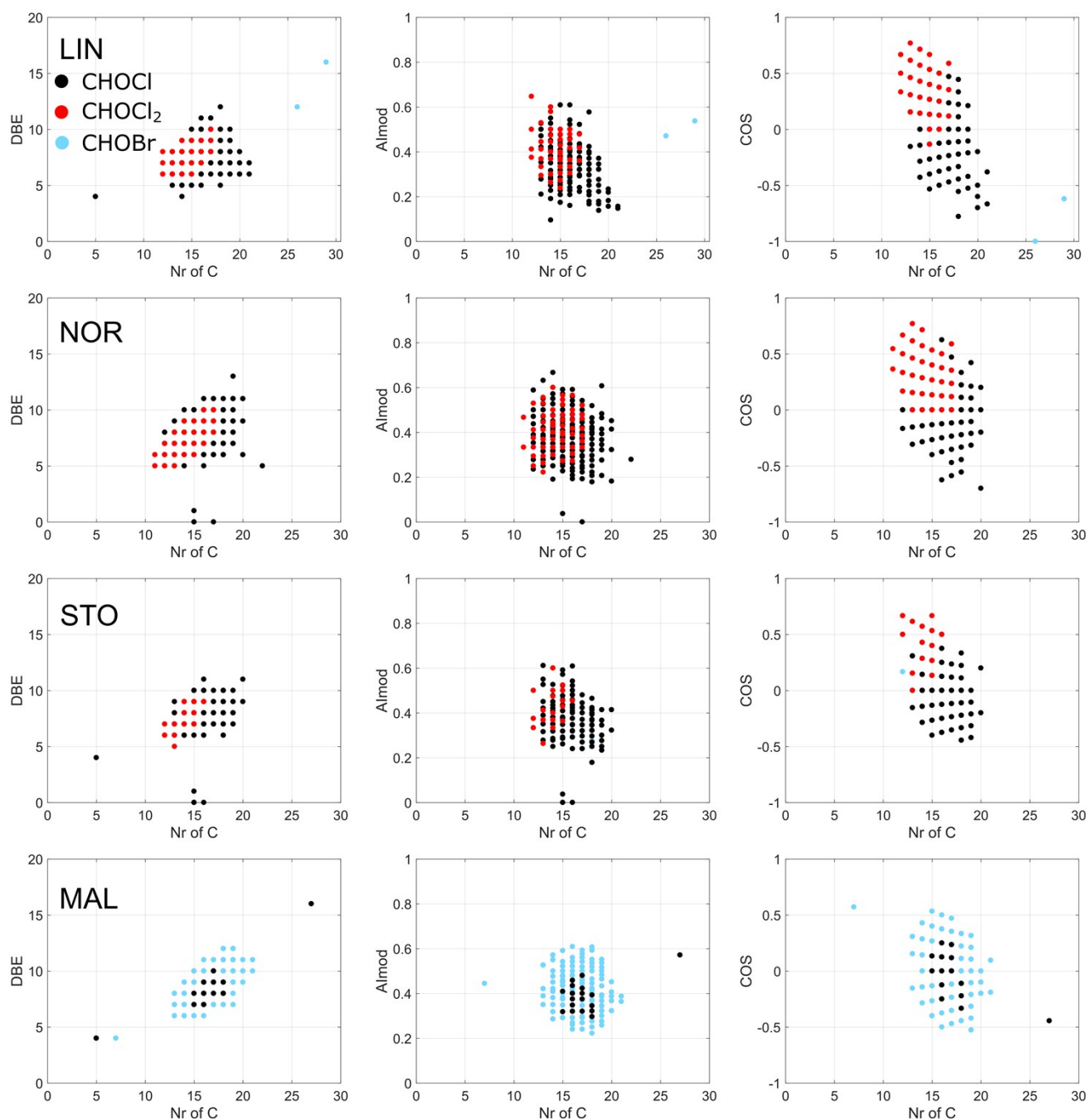


Fig. S1 Plots showing counts of DBE, Al_{mod} and COS versus number of carbon for verified DBPs formed in the four waterworks (DBPs formed throughout the five sampling events combined).

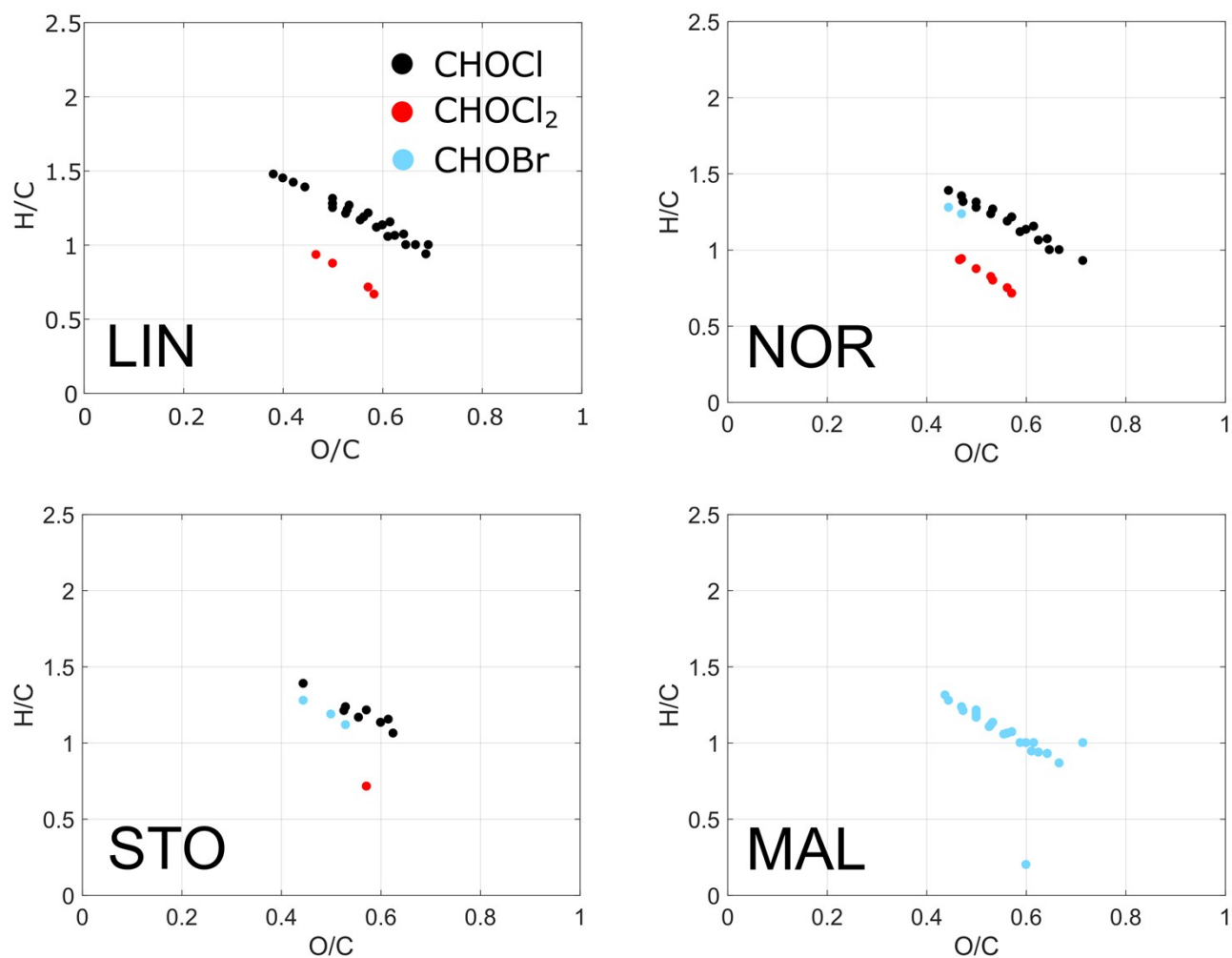


Fig. S2 Van Krevelen plots for verified DBPs with Kendrick mass defect, $-KMD/z^*$ above 0.15 for verified DBPs formed in the four waterworks (DBPs formed throughout the five sampling events combined).

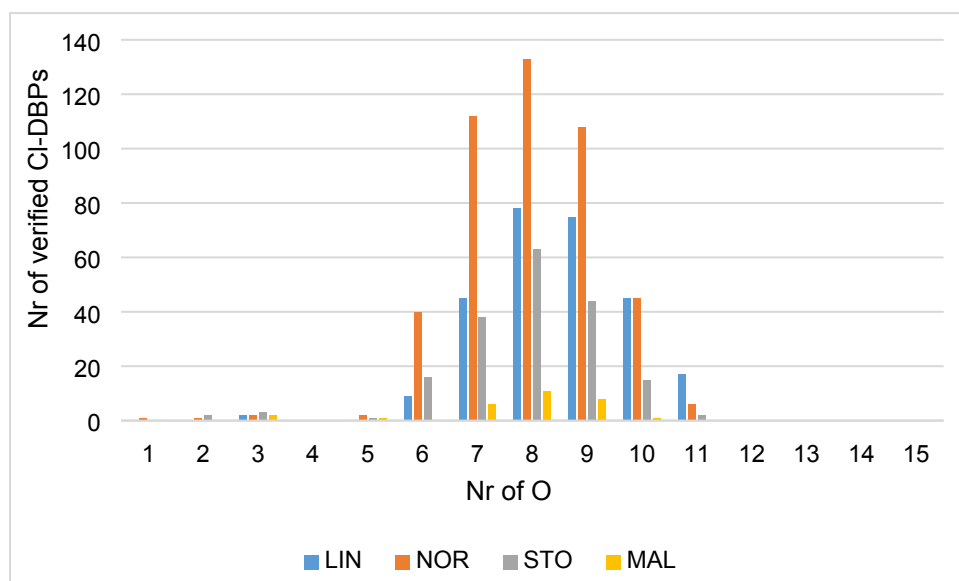


Fig. S3 The number of verified chlorinated DBPs (CHO-type) formed in the four waterworks plotted against the number of oxygen atoms of each DBP composition (DBPs formed throughout the five sampling events combined).

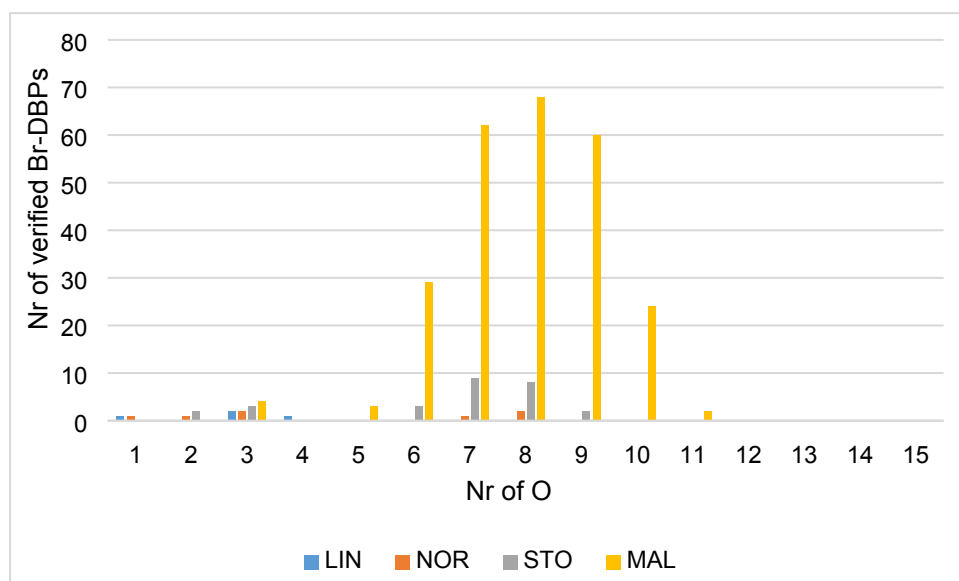


Fig. S4 The number of verified brominated DBPs (CHO-type) formed in the four waterworks plotted against the number of oxygen atoms of each DBP composition (DBPs formed throughout the five sampling events combined).

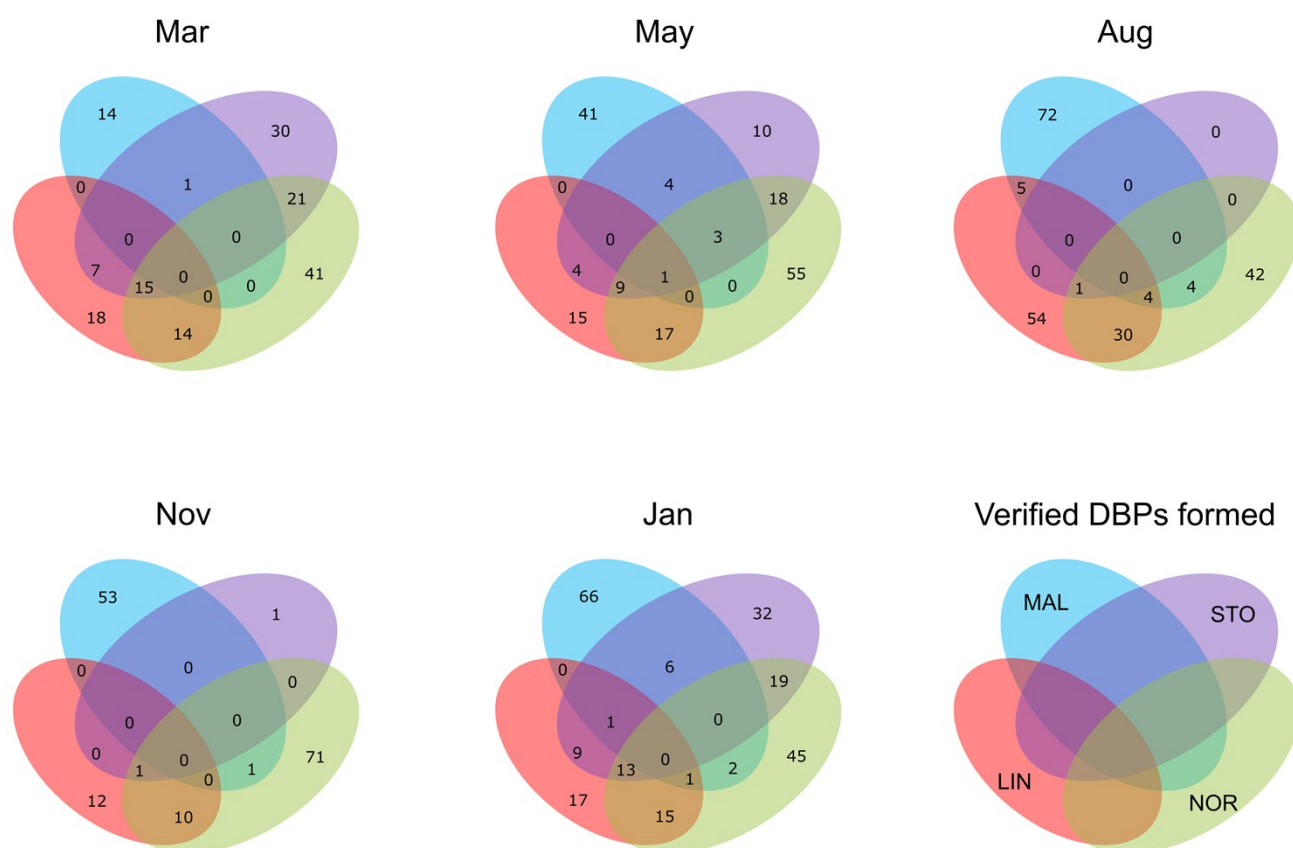


Fig. S5 Venn diagrams showing the number of unique and shared verified molecular compositions of DBPs formed in the four waterworks at the five different months of sampling. Few DBPs were verified for STO in Aug and Nov due to low spectral intensities for those samples.

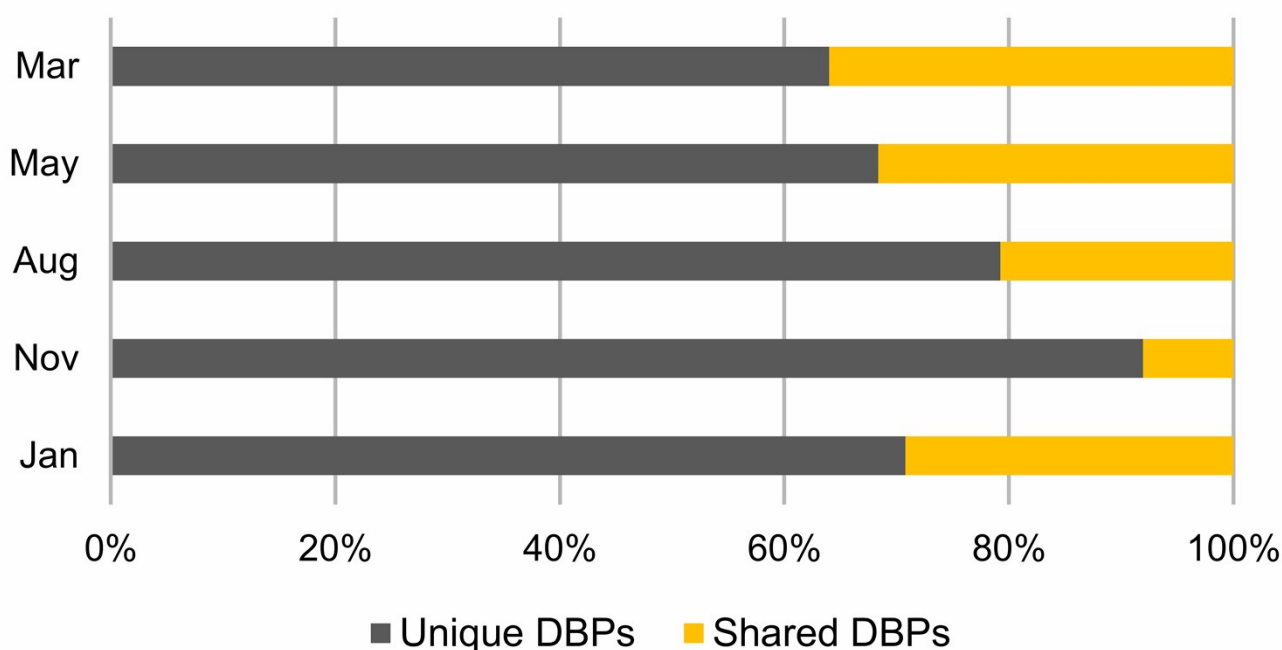


Fig. S6 Percentage of unique and shared verified DBPs formed in the four waterworks at the five different months of sampling.

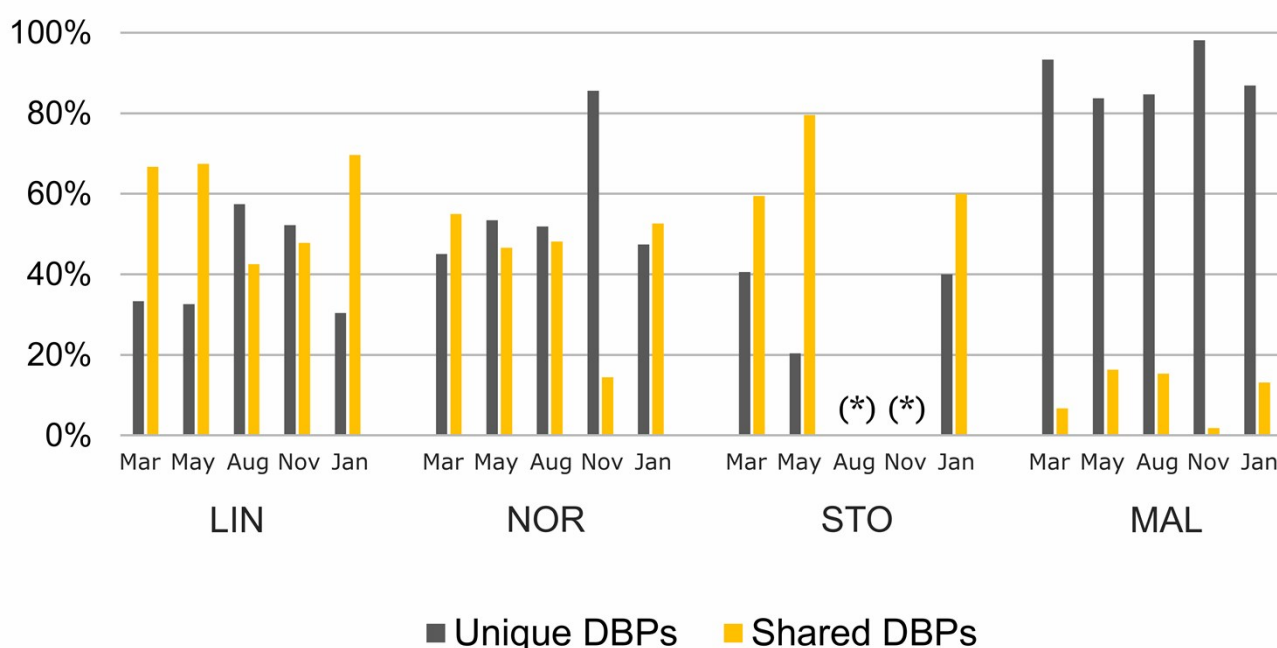


Fig. S7 Percentage of unique and shared verified DBPs formed each month in the four waterworks respectively. (*) Few DBPs were verified for STO in Aug and Nov due to low spectral intensities for those samples.

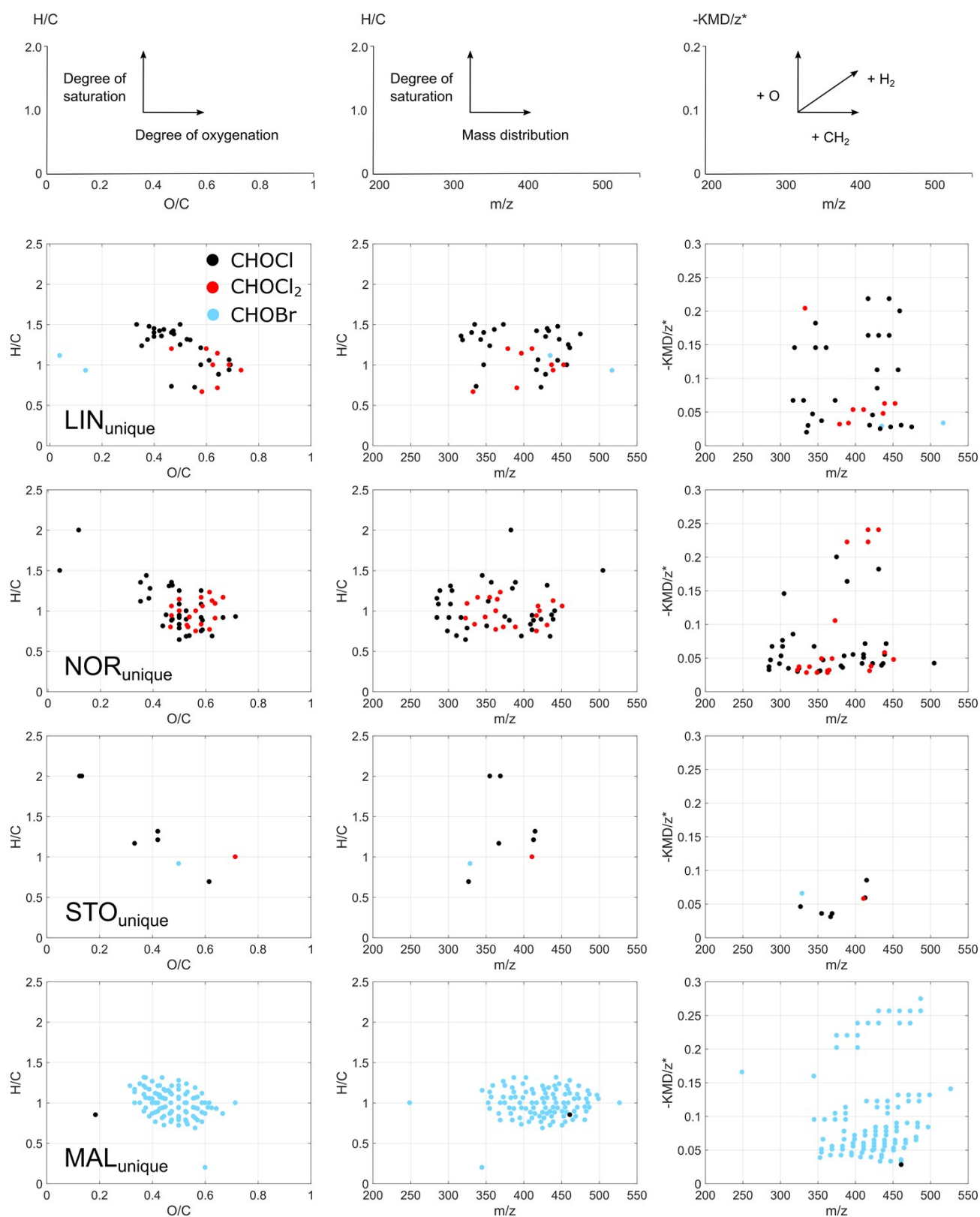


Fig. S8 Van Krevelen, H/C to mass and modified Kendrick mass plots comprising the verified unique DBPs formed in the four waterworks (DBPs formed throughout the five sampling events combined).

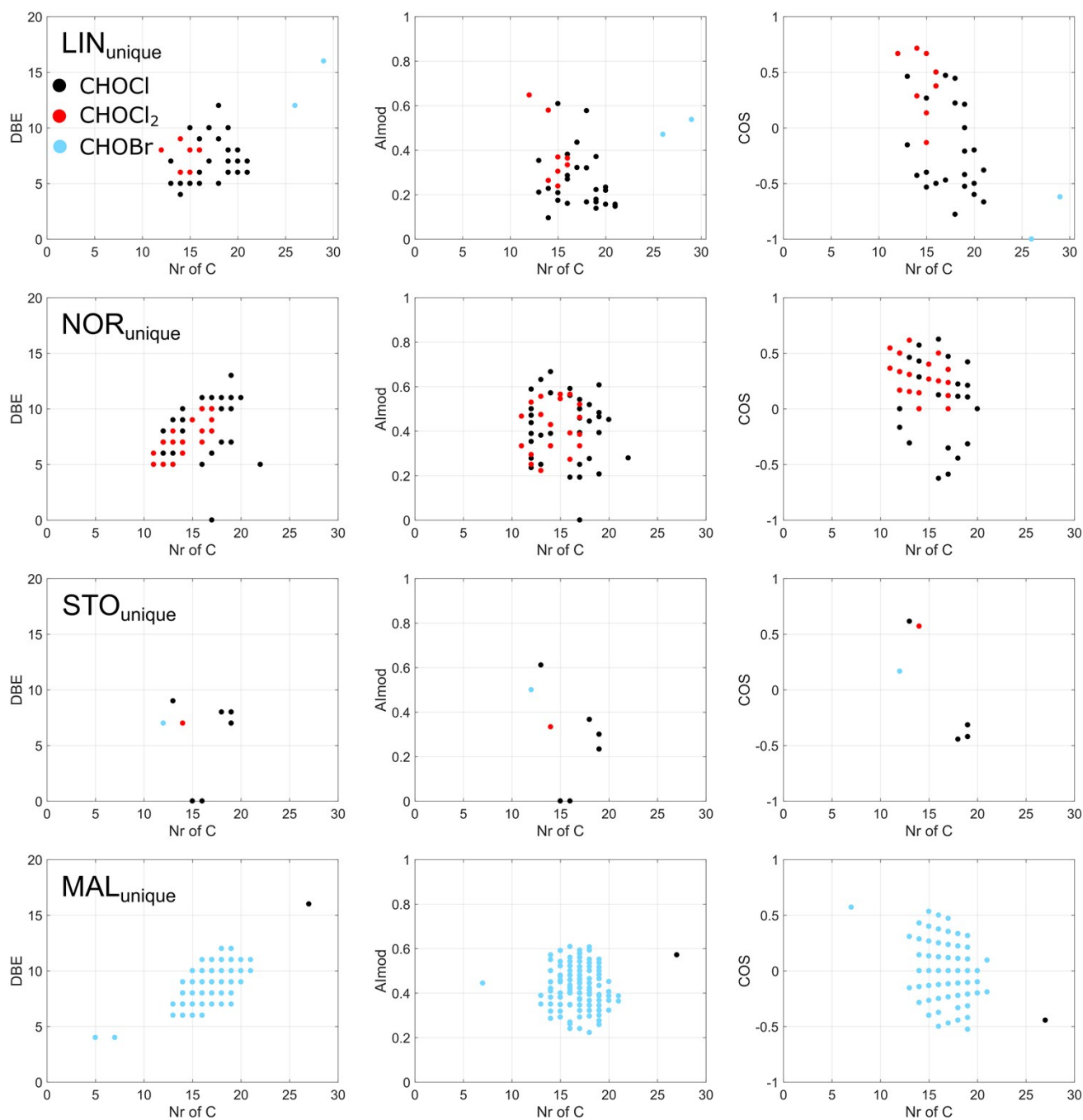


Fig. S9 Plots showing counts of DBE, AI_{mod} and C_{OS} versus number of carbon for unique verified DBPs formed in the four waterworks (DBPs formed throughout the five sampling events combined).

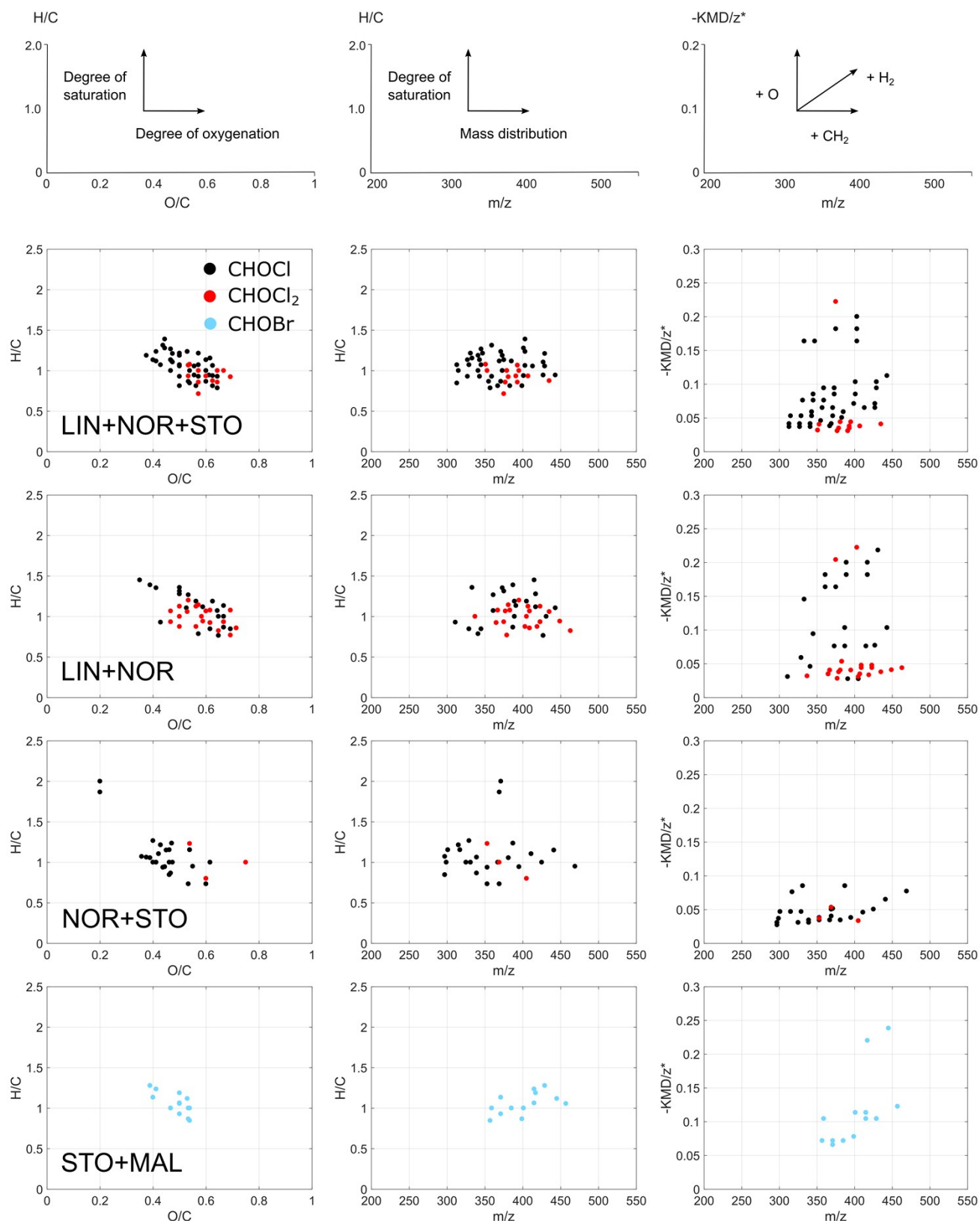


Fig. S10 Van Krevelen, H/C to mass and modified Kendrick mass plots for the verified DBPs shared between LIN, NOR and STO, LIN and NOR, NOR and STO and STO and MAL, respectively (DBPs formed throughout the five sampling events combined).

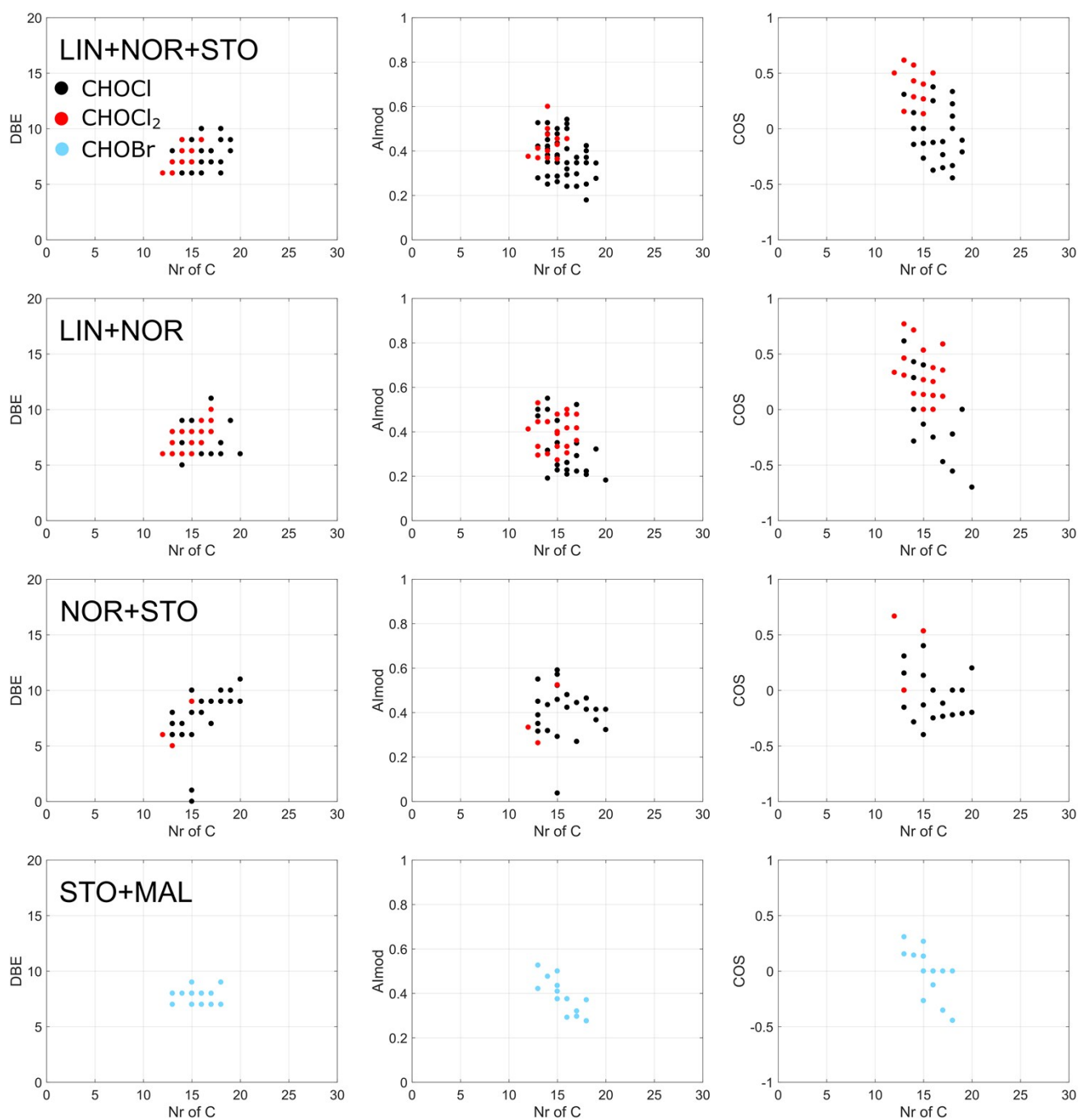


Fig. S11 Plots showing counts of DBE, AI_{mod} and C_{OS} versus number of carbon for the verified DBPs shared between LIN, NOR and STO, LIN and NOR, NOR and STO and STO and MAL respectively (DBPs formed throughout the five sampling events combined).

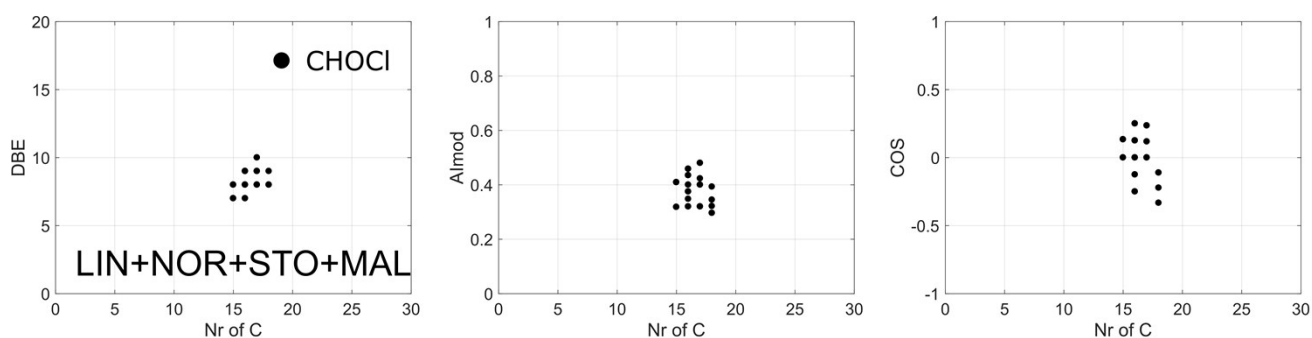


Fig. S12 Plots showing counts of DBE, AI_{mod} and C_{OS} versus number of carbon for verified DBPs shared between all four waterworks (DBPs formed throughout the five sampling events combined).

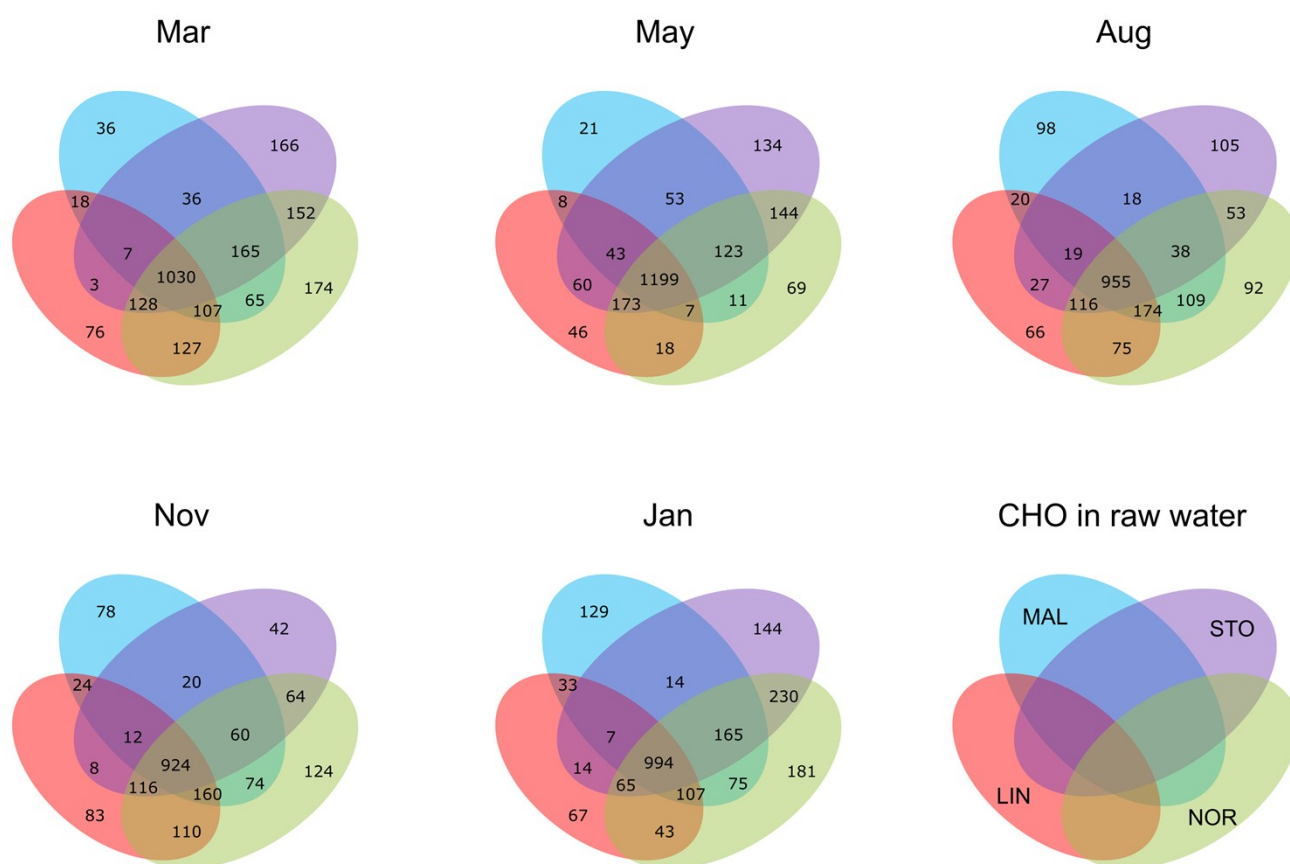


Fig. S13 Venn diagrams showing the number of unique and shared CHO molecular compositions in the raw waters of the four waterworks at the five different months of sampling.

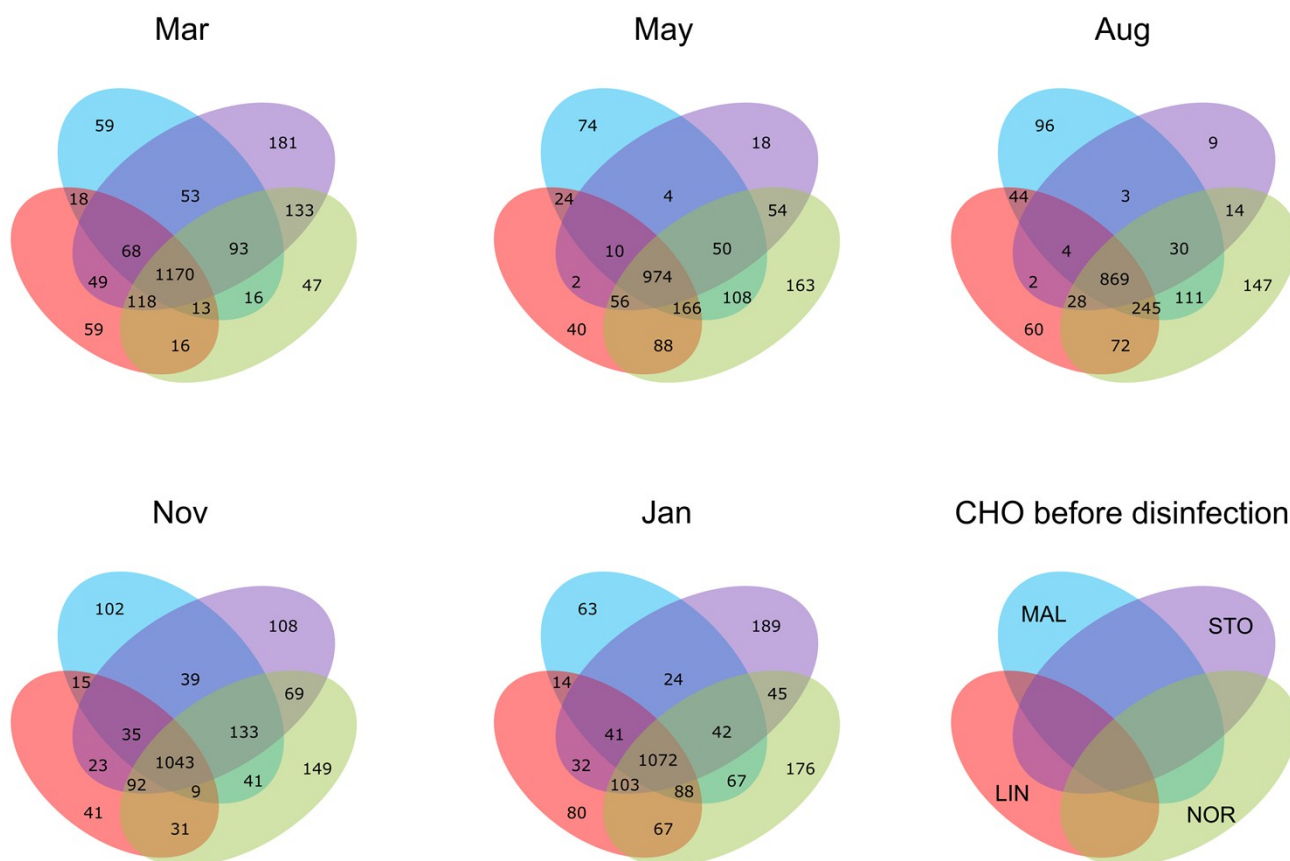


Fig. S14 Venn diagrams showing the number of unique and shared CHO molecular compositions present before chemical disinfection in the four waterworks at the five different months of sampling.

Table S1 Summary of verified DBP molecular compositions formed in the four waterworks (DBPs formed throughout the five sampling events combined). DBPs were often detected more than at one sampling occasion but each DBP formula is just reported one time in this overview list.

WTP	DBP Formula Neutral form	Theoretical Mass Negative Ion
LIN	C12 H10 O8 Cl2	350.968
LIN	C12 H12 O7 Cl2	336.98874
LIN	C12 H12 O8 Cl2	352.98365
LIN	C12 H8 O7 Cl2	332.95744
LIN	C13 H10 O9 Cl2	378.96292
LIN	C13 H11 O7 Cl1	313.01206
LIN	C13 H11 O8 Cl1	329.00697
LIN	C13 H11 O9 Cl1	345.00189
LIN	C13 H12 O8 Cl2	364.98365
LIN	C13 H12 O9 Cl2	380.97857
LIN	C13 H13 O7 Cl1	315.02771
LIN	C13 H13 O9 Cl1	347.01754
LIN	C13 H14 O7 Cl2	351.00439
LIN	C13 H14 O8 Cl2	366.9993
LIN	C13 H14 O9 Cl2	382.99422
LIN	C13 H15 O8 Cl1	333.03827
LIN	C13 H17 O7 Cl1	319.05901
LIN	C14 H10 O8 Cl2	374.968
LIN	C14 H10 O9 Cl2	390.96292
LIN	C14 H11 O8 Cl1	341.00697
LIN	C14 H11 O9 Cl1	357.00189
LIN	C14 H12 O10 Cl2	408.97348
LIN	C14 H12 O8 Cl2	376.98365
LIN	C14 H12 O9 Cl2	392.97857
LIN	C14 H13 O6 Cl1	311.03279
LIN	C14 H13 O7 Cl1	327.02771
LIN	C14 H13 O8 Cl1	343.02262
LIN	C14 H13 O9 Cl1	359.01754
LIN	C14 H14 O8 Cl2	378.9993
LIN	C14 H14 O9 Cl2	394.99422
LIN	C14 H15 O10 Cl1	377.0281
LIN	C14 H15 O6 Cl1	313.04844
LIN	C14 H15 O7 Cl1	329.04336
LIN	C14 H15 O8 Cl1	345.03827
LIN	C14 H15 O9 Cl1	361.03319
LIN	C14 H16 O8 Cl2	381.01495
LIN	C14 H16 O9 Cl2	397.00987
LIN	C14 H17 O7 Cl1	331.05901
LIN	C14 H17 O8 Cl1	347.05392
LIN	C14 H19 O6 Cl1	317.07974

LIN	C14 H19 O7 Cl1	333.07466
LIN	C14 H21 O7 Cl1	335.09031
LIN	C15 H11 O7 Cl1	337.01206
LIN	C15 H12 O10 Cl2	420.97348
LIN	C15 H13 O10 Cl1	387.01245
LIN	C15 H13 O8 Cl1	355.02262
LIN	C15 H13 O9 Cl1	371.01754
LIN	C15 H14 O10 Cl2	422.98913
LIN	C15 H14 O11 Cl2	438.98405
LIN	C15 H14 O7 Cl2	375.00439
LIN	C15 H14 O8 Cl2	390.9993
LIN	C15 H14 O9 Cl2	406.99422
LIN	C15 H15 O10 Cl1	389.0281
LIN	C15 H15 O7 Cl1	341.04336
LIN	C15 H15 O8 Cl1	357.03827
LIN	C15 H15 O9 Cl1	373.03319
LIN	C15 H16 O7 Cl2	377.02004
LIN	C15 H16 O8 Cl2	393.01495
LIN	C15 H16 O9 Cl2	409.00987
LIN	C15 H17 O10 Cl1	391.04375
LIN	C15 H17 O6 Cl1	327.06409
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LIN	C15 H18 O7 Cl2	379.03569
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NOR	C20 H23 O9 Cl1	441.09579
NOR	C20 H29 O7 Cl1	415.15291
NOR	C22 H33 O1 Cl1 Br2	505.05139
STO	C12 H10 O8 Cl2	350.968
STO	C12 H11 O6 Br1	328.96663
STO	C12 H12 O8 Cl2	352.98365
STO	C12 H12 O9 Cl2	368.97857
STO	C13 H11 O6 Cl1	297.01714
STO	C13 H11 O7 Br1	356.96154
STO	C13 H11 O7 Cl1	313.01206
STO	C13 H12 O9 Cl2	380.97857
STO	C13 H13 O6 Cl1	299.03279
STO	C13 H13 O7 Br1	358.97719
STO	C13 H13 O7 Cl1	315.02771
STO	C13 H13 O8 Cl1	331.02262
STO	C13 H14 O7 Cl2	351.00439
STO	C13 H15 O6 Cl1	301.04844
STO	C13 H15 O7 Cl1	317.04336
STO	C13 H15 O8 Cl1	333.03827

STO	C13 H16 O7 Cl2	353.02004
STO	C13 H9 O8 Cl1	326.99132
STO	C14 H10 O8 Cl2	374.968
STO	C14 H11 O9 Cl1	357.00189
STO	C14 H12 O8 Cl2	376.98365
STO	C14 H12 O9 Cl2	392.97857
STO	C14 H13 O7 Br1	370.97719
STO	C14 H13 O7 Cl1	327.02771
STO	C14 H13 O8 Cl1	343.02262
STO	C14 H13 O9 Cl1	359.01754
STO	C14 H14 O10 Cl2	410.98913
STO	C14 H14 O8 Cl2	378.9993
STO	C14 H14 O9 Cl2	394.99422
STO	C14 H15 O10 Cl1	377.0281
STO	C14 H15 O5 Cl1	297.05353
STO	C14 H15 O6 Cl1	313.04844
STO	C14 H15 O7 Cl1	329.04336
STO	C14 H15 O8 Cl1	345.03827
STO	C14 H17 O6 Cl1	315.06409
STO	C14 H17 O7 Cl1	331.05901
STO	C14 H17 O8 Cl1	347.05392
STO	C15 H11 O8 Cl1	353.00697
STO	C15 H11 O9 Cl1	369.00189
STO	C15 H12 O10 Cl2	420.97348
STO	C15 H12 O9 Cl2	404.97857
STO	C15 H13 O7 Cl1	339.02771
STO	C15 H13 O8 Br1	398.97211
STO	C15 H13 O8 Cl1	355.02262
STO	C15 H13 O9 Cl1	371.01754
STO	C15 H14 O8 Cl2	390.9993
STO	C15 H14 O9 Cl2	406.99422
STO	C15 H15 O6 Cl1	325.04844
STO	C15 H15 O7 Br1	384.99284
STO	C15 H15 O7 Cl1	341.04336
STO	C15 H15 O8 Br1	400.98776
STO	C15 H15 O8 Cl1	357.03827
STO	C15 H15 O9 Cl1	373.03319
STO	C15 H16 O8 Cl2	393.01495
STO	C15 H17 O6 Br1	371.01358
STO	C15 H17 O6 Cl1	327.06409
STO	C15 H17 O7 Cl1	343.05901
STO	C15 H17 O8 Cl1	359.05392
STO	C15 H17 O9 Cl1	375.04884
STO	C15 H19 O6 Cl1	329.07974
STO	C15 H19 O7 Cl1	345.07466
STO	C15 H28 O3 Cl1 Br1	369.08376

STO	C15 H30 O2 Cl1 Br1	355.1045
STO	C15 H30 O3 Cl1 Br1	371.09941
STO	C16 H11 O9 Cl1	381.00189
STO	C16 H13 O10 Cl1	399.01245
STO	C16 H13 O8 Cl1	367.02262
STO	C16 H13 O9 Cl1	383.01754
STO	C16 H14 O10 Cl2	434.98913
STO	C16 H15 O10 Cl1	401.0281
STO	C16 H15 O7 Cl1	353.04336
STO	C16 H15 O8 Cl1	369.03827
STO	C16 H15 O9 Cl1	385.03319
STO	C16 H17 O10 Cl1	403.04375
STO	C16 H17 O6 Cl1	339.06409
STO	C16 H17 O7 Cl1	355.05901
STO	C16 H17 O8 Br1	415.00341
STO	C16 H17 O8 Cl1	371.05392
STO	C16 H17 O9 Cl1	387.04884
STO	C16 H19 O6 Cl1	341.07974
STO	C16 H19 O7 Cl1	357.07466
STO	C16 H19 O8 Br1	417.01906
STO	C16 H19 O8 Cl1	373.06957
STO	C16 H21 O7 Cl1	359.09031
STO	C16 H32 O2 Cl1 Br1	369.12015
STO	C17 H15 O9 Cl1	397.03319
STO	C17 H17 O7 Cl1	367.05901
STO	C17 H17 O8 Cl1	383.05392
STO	C17 H17 O9 Cl1	399.04884
STO	C17 H19 O7 Cl1	369.07466
STO	C17 H19 O8 Cl1	385.06957
STO	C17 H19 O9 Br1	445.01397
STO	C17 H19 O9 Cl1	401.06449
STO	C17 H21 O7 Br1	415.03979
STO	C17 H21 O7 Cl1	371.09031
STO	C17 H21 O8 Cl1	387.08522
STO	C17 H21 O9 Cl1	403.08014
STO	C18 H17 O10 Cl1	427.04375
STO	C18 H17 O11 Cl1	443.03867
STO	C18 H17 O8 Cl1	395.05392
STO	C18 H19 O10 Cl1	429.0594
STO	C18 H19 O7 Cl1	381.07466
STO	C18 H19 O8 Cl1	397.06957
STO	C18 H19 O9 Br1	457.01397
STO	C18 H19 O9 Cl1	413.06449
STO	C18 H21 O10 Cl1	431.07505
STO	C18 H21 O6 Cl1	367.09539
STO	C18 H21 O7 Cl1	383.09031

STO	C18 H21 O8 Cl1	399.08522
STO	C18 H21 O9 Cl1	415.08014
STO	C18 H23 O7 Br1	429.05544
STO	C18 H23 O8 Br1	445.05036
STO	C18 H23 O8 Cl1	401.10087
STO	C18 H25 O8 Cl1	403.11652
STO	C19 H19 O9 Cl1	425.06449
STO	C19 H21 O8 Cl1	411.08522
STO	C19 H21 O9 Cl1	427.08014
STO	C19 H23 O10 Cl1	445.0907
STO	C19 H23 O8 Cl1	413.10087
STO	C19 H23 O9 Cl1	429.09579
STO	C19 H25 O8 Cl1	415.11652
STO	C20 H19 O11 Cl1	469.05432
STO	C20 H23 O9 Cl1	441.09579
STO	C5 H1 O3 Cl1 Br2	300.79082
MAL	C13 H11 O7 Br1	356.96154
MAL	C13 H13 O7 Br1	358.97719
MAL	C13 H13 O8 Br1	374.97211
MAL	C13 H15 O6 Br1	344.99793
MAL	C14 H11 O7 Br1	368.96154
MAL	C14 H11 O8 Br1	384.95646
MAL	C14 H13 O6 Br1	354.98228
MAL	C14 H13 O7 Br1	370.97719
MAL	C14 H13 O8 Br1	386.97211
MAL	C14 H13 O9 Br1	402.96702
MAL	C14 H15 O6 Br1	356.99793
MAL	C14 H15 O7 Br1	372.99284
MAL	C14 H15 O8 Br1	388.98776
MAL	C14 H17 O6 Br1	359.01358
MAL	C14 H17 O7 Br1	375.00849
MAL	C15 H11 O8 Br1	396.95646
MAL	C15 H13 O10 Br1	430.96194
MAL	C15 H13 O6 Br1	366.98228
MAL	C15 H13 O7 Br1	382.97719
MAL	C15 H13 O8 Br1	398.97211
MAL	C15 H13 O9 Br1	414.96702
MAL	C15 H15 O5 Br1	353.00301
MAL	C15 H15 O6 Br1	368.99793
MAL	C15 H15 O7 Br1	384.99284
MAL	C15 H15 O8 Br1	400.98776
MAL	C15 H15 O8 Cl1	357.03827
MAL	C15 H15 O9 Br1	416.98267
MAL	C15 H17 O5 Br1	355.01866
MAL	C15 H17 O6 Br1	371.01358
MAL	C15 H17 O7 Br1	387.00849

MAL	C15 H17 O8 BrI	403.00341
MAL	C15 H17 O8 ClI	359.05392
MAL	C15 H19 O6 BrI	373.02923
MAL	C16 H11 O9 BrI	424.95137
MAL	C16 H13 O7 BrI	394.97719
MAL	C16 H13 O8 BrI	410.97211
MAL	C16 H13 O9 BrI	426.96702
MAL	C16 H15 O10 BrI	444.97759
MAL	C16 H15 O6 BrI	380.99793
MAL	C16 H15 O7 BrI	396.99284
MAL	C16 H15 O8 BrI	412.98776
MAL	C16 H15 O8 ClI	369.03827
MAL	C16 H15 O9 BrI	428.98267
MAL	C16 H15 O9 ClI	385.03319
MAL	C16 H17 O6 BrI	383.01358
MAL	C16 H17 O7 BrI	399.00849
MAL	C16 H17 O7 ClI	355.05901
MAL	C16 H17 O8 BrI	415.00341
MAL	C16 H17 O8 ClI	371.05392
MAL	C16 H17 O9 BrI	430.99832
MAL	C16 H17 O9 ClI	387.04884
MAL	C16 H19 O6 BrI	385.02923
MAL	C16 H19 O7 BrI	401.02414
MAL	C16 H19 O7 ClI	357.07466
MAL	C16 H19 O8 BrI	417.01906
MAL	C16 H19 O9 BrI	433.01397
MAL	C16 H21 O6 BrI	387.04488
MAL	C16 H21 O7 BrI	403.03979
MAL	C17 H13 O10 BrI	454.96194
MAL	C17 H13 O7 BrI	406.97719
MAL	C17 H13 O8 BrI	422.97211
MAL	C17 H13 O9 BrI	438.96702
MAL	C17 H15 O10 BrI	456.97759
MAL	C17 H15 O7 BrI	408.99284
MAL	C17 H15 O8 BrI	424.98776
MAL	C17 H15 O9 BrI	440.98267
MAL	C17 H15 O9 ClI	397.03319
MAL	C17 H17 O10 BrI	458.99324
MAL	C17 H17 O10 ClI	415.04375
MAL	C17 H17 O6 BrI	395.01358
MAL	C17 H17 O7 BrI	411.00849
MAL	C17 H17 O8 BrI	427.00341
MAL	C17 H17 O8 ClI	383.05392
MAL	C17 H17 O9 BrI	442.99832
MAL	C17 H17 O9 ClI	399.04884
MAL	C17 H19 O10 BrI	461.00889

MAL	C17 H19 O7 Brl	413.02414
MAL	C17 H19 O8 Brl	429.01906
MAL	C17 H19 O9 Brl	445.01397
MAL	C17 H19 O9 Cl1	401.06449
MAL	C17 H21 O6 Brl	399.04488
MAL	C17 H21 O7 Brl	415.03979
MAL	C17 H21 O8 Brl	431.03471
MAL	C17 H21 O9 Brl	447.02962
MAL	C18 H13 O8 Brl	434.97211
MAL	C18 H13 O9 Brl	450.96702
MAL	C18 H15 O10 Brl	468.97759
MAL	C18 H15 O7 Brl	420.99284
MAL	C18 H15 O8 Brl	436.98776
MAL	C18 H15 O9 Brl	452.98267
MAL	C18 H17 O10 Brl	470.99324
MAL	C18 H17 O11 Brl	486.98815
MAL	C18 H17 O8 Brl	439.00341
MAL	C18 H17 O9 Brl	454.99832
MAL	C18 H19 O10 Brl	473.00889
MAL	C18 H19 O7 Brl	425.02414
MAL	C18 H19 O8 Brl	441.01906
MAL	C18 H19 O8 Cl1	397.06957
MAL	C18 H19 O9 Brl	457.01397
MAL	C18 H21 O6 Brl	411.04488
MAL	C18 H21 O7 Brl	427.03979
MAL	C18 H21 O7 Cl1	383.09031
MAL	C18 H21 O8 Brl	443.03471
MAL	C18 H21 O8 Cl1	399.08522
MAL	C18 H21 O9 Brl	459.02962
MAL	C18 H21 O9 Cl1	415.08014
MAL	C18 H23 O7 Brl	429.05544
MAL	C18 H23 O8 Brl	445.05036
MAL	C18 H23 O9 Brl	461.04527
MAL	C19 H15 O10 Brl	480.97759
MAL	C19 H15 O9 Brl	464.98267
MAL	C19 H17 O10 Brl	482.99324
MAL	C19 H17 O7 Brl	435.00849
MAL	C19 H17 O8 Brl	451.00341
MAL	C19 H17 O9 Brl	466.99832
MAL	C19 H19 O10 Brl	485.00889
MAL	C19 H19 O8 Brl	453.01906
MAL	C19 H21 O10 Brl	487.02454
MAL	C19 H21 O7 Brl	439.03979
MAL	C19 H21 O8 Brl	455.03471
MAL	C19 H21 O9 Brl	471.02962
MAL	C19 H23 O6 Brl	425.06053

MAL	C19 H23 O7 Br1	441.05544
MAL	C19 H23 O8 Br1	457.05036
MAL	C19 H23 O9 Br1	473.04527
MAL	C19 H25 O7 Br1	443.07109
MAL	C20 H19 O9 Br1	481.01397
MAL	C20 H21 O10 Br1	499.02454
MAL	C20 H21 O8 Br1	467.03471
MAL	C20 H21 O9 Br1	483.02962
MAL	C20 H23 O9 Br1	485.04527
MAL	C21 H21 O11 Br1	527.01945
MAL	C21 H23 O9 Br1	497.04527
MAL	C27 H23 O5 Cl1	461.11613
MAL	C5 H1 O3 Br3	344.74031
MAL	C5 H1 O3 Cl1 Br2	300.79082
MAL	C7 H7 O5 Br1	248.94041

Table S2 Summary of DBP formulae that were unique and shared between the waterworks (DBPs formed throughout the five sampling events combined).

Water treatment plants where DBP formula was detected	DBP Formula Neutral form	Theoretical Mass Negative Ion
LIN-unique	C12 H8 O7 Cl2	332.95744
LIN-unique	C13 H13 O9 Cl1	347.01754
LIN-unique	C13 H17 O7 Cl1	319.05901
LIN-unique	C14 H10 O9 Cl2	390.96292
LIN-unique	C14 H16 O9 Cl2	397.00987
LIN-unique	C14 H19 O6 Cl1	317.07974
LIN-unique	C14 H21 O7 Cl1	335.09031
LIN-unique	C15 H11 O7 Cl1	337.01206
LIN-unique	C15 H14 O11 Cl2	438.98405
LIN-unique	C15 H18 O7 Cl2	379.03569
LIN-unique	C15 H18 O9 Cl2	411.02552
LIN-unique	C15 H21 O6 Cl1	331.09539
LIN-unique	C15 H21 O7 Cl1	347.09031
LIN-unique	C16 H15 O11 Cl1	417.02302
LIN-unique	C16 H16 O10 Cl2	437.00478
LIN-unique	C16 H16 O11 Cl2	452.9997
LIN-unique	C16 H17 O11 Cl1	419.03867
LIN-unique	C16 H21 O6 Cl1	343.09539
LIN-unique	C16 H23 O7 Cl1	361.10596
LIN-unique	C17 H15 O11 Cl1	429.02302
LIN-unique	C17 H21 O6 Cl1	355.09539
LIN-unique	C18 H13 O10 Cl1	423.01245
LIN-unique	C18 H19 O11 Cl1	445.05432
LIN-unique	C18 H27 O6 Cl1	373.14234
LIN-unique	C19 H19 O11 Cl1	457.05432
LIN-unique	C19 H23 O11 Cl1	461.08562
LIN-unique	C19 H25 O10 Cl1	447.10635
LIN-unique	C19 H27 O8 Cl1	417.13217
LIN-unique	C19 H27 O9 Cl1	433.12709
LIN-unique	C20 H25 O10 Cl1	459.10635
LIN-unique	C20 H27 O8 Cl1	429.13217
LIN-unique	C20 H29 O8 Cl1	431.14782
LIN-unique	C21 H29 O10 Cl1	475.13765
LIN-unique	C21 H31 O8 Cl1	445.16347
LIN-unique	C26 H29 O1 Br1	435.1329
LIN-unique	C29 H27 O4 Br1	517.102
NOR-unique	C11 H10 O7 Cl2	322.97309
NOR-unique	C11 H12 O7 Cl2	324.98874
NOR-unique	C12 H10 O7 Cl2	334.97309
NOR-unique	C12 H11 O6 Cl1	285.01714
NOR-unique	C12 H11 O7 Cl1	301.01206

NOR-unique	C12 H11 O8 Cl1	317.00697
NOR-unique	C12 H13 O6 Cl1	287.03279
NOR-unique	C12 H13 O7 Cl1	303.02771
NOR-unique	C12 H14 O7 Cl2	339.00439
NOR-unique	C12 H14 O8 Cl2	354.9993
NOR-unique	C12 H15 O6 Cl1	289.04844
NOR-unique	C12 H15 O7 Cl1	305.04336
NOR-unique	C12 H9 O7 Cl1	298.99641
NOR-unique	C13 H10 O8 Cl2	362.968
NOR-unique	C13 H12 O7 Cl2	348.98874
NOR-unique	C13 H15 O5 Cl1	285.05353
NOR-unique	C13 H16 O8 Cl2	369.01495
NOR-unique	C13 H17 O6 Cl1	303.06409
NOR-unique	C13 H9 O7 Cl1	310.99641
NOR-unique	C14 H11 O7 Cl1	325.01206
NOR-unique	C14 H13 O10 Cl1	375.01245
NOR-unique	C14 H14 O7 Cl2	363.00439
NOR-unique	C14 H16 O7 Cl2	365.02004
NOR-unique	C14 H9 O7 Cl1	322.99641
NOR-unique	C15 H12 O7 Cl2	372.98874
NOR-unique	C15 H12 O8 Cl2	388.98365
NOR-unique	C16 H11 O10 Cl1	396.9968
NOR-unique	C16 H12 O9 Cl2	416.97857
NOR-unique	C16 H13 O7 Cl1	351.02771
NOR-unique	C16 H16 O9 Cl2	421.00987
NOR-unique	C16 H18 O10 Cl2	439.02043
NOR-unique	C16 H23 O6 Cl1	345.11104
NOR-unique	C17 H13 O10 Cl1	411.01245
NOR-unique	C17 H14 O9 Cl2	430.99422
NOR-unique	C17 H15 O10 Cl1	413.0281
NOR-unique	C17 H15 O8 Cl1	381.03827
NOR-unique	C17 H16 O8 Cl2	417.01495
NOR-unique	C17 H18 O10 Cl2	451.02043
NOR-unique	C17 H18 O8 Cl2	419.0306
NOR-unique	C17 H19 O6 Cl1	353.07974
NOR-unique	C17 H23 O6 Cl1	357.11104
NOR-unique	C17 H23 O8 Cl1	389.10087
NOR-unique	C17 H34 O2 Cl1 Br1	383.1358
NOR-unique	C18 H15 O9 Cl1	409.03319
NOR-unique	C18 H17 O9 Cl1	411.04884
NOR-unique	C18 H23 O7 Cl1	385.10596
NOR-unique	C19 H13 O10 Cl1	435.01245
NOR-unique	C19 H17 O10 Cl1	439.04375
NOR-unique	C19 H17 O9 Cl1	423.04884
NOR-unique	C19 H19 O10 Cl1	441.0594
NOR-unique	C19 H25 O9 Cl1	431.11144

NOR-unique	C20 H19 O9 Cl1	437.06449
NOR-unique	C22 H33 O1 Cl1 Br2	505.05139
STO-unique	C12 H11 O6 Br1	328.96663
STO-unique	C13 H9 O8 Cl1	326.99132
STO-unique	C14 H14 O10 Cl2	410.98913
STO-unique	C15 H30 O2 Cl1 Br1	355.1045
STO-unique	C16 H32 O2 Cl1 Br1	369.12015
STO-unique	C18 H21 O6 Cl1	367.09539
STO-unique	C19 H23 O8 Cl1	413.10087
STO-unique	C19 H25 O8 Cl1	415.11652
MAL-unique	C13 H13 O8 Br1	374.97211
MAL-unique	C13 H15 O6 Br1	344.99793
MAL-unique	C14 H11 O7 Br1	368.96154
MAL-unique	C14 H11 O8 Br1	384.95646
MAL-unique	C14 H13 O6 Br1	354.98228
MAL-unique	C14 H13 O8 Br1	386.97211
MAL-unique	C14 H13 O9 Br1	402.96702
MAL-unique	C14 H15 O6 Br1	356.99793
MAL-unique	C14 H15 O7 Br1	372.99284
MAL-unique	C14 H15 O8 Br1	388.98776
MAL-unique	C14 H17 O6 Br1	359.01358
MAL-unique	C14 H17 O7 Br1	375.00849
MAL-unique	C15 H11 O8 Br1	396.95646
MAL-unique	C15 H13 O10 Br1	430.96194
MAL-unique	C15 H13 O6 Br1	366.98228
MAL-unique	C15 H13 O7 Br1	382.97719
MAL-unique	C15 H13 O9 Br1	414.96702
MAL-unique	C15 H15 O5 Br1	353.00301
MAL-unique	C15 H15 O6 Br1	368.99793
MAL-unique	C15 H15 O9 Br1	416.98267
MAL-unique	C15 H17 O5 Br1	355.01866
MAL-unique	C15 H17 O7 Br1	387.00849
MAL-unique	C15 H17 O8 Br1	403.00341
MAL-unique	C15 H19 O6 Br1	373.02923
MAL-unique	C16 H11 O9 Br1	424.95137
MAL-unique	C16 H13 O7 Br1	394.97719
MAL-unique	C16 H13 O8 Br1	410.97211
MAL-unique	C16 H13 O9 Br1	426.96702
MAL-unique	C16 H15 O10 Br1	444.97759
MAL-unique	C16 H15 O6 Br1	380.99793
MAL-unique	C16 H15 O7 Br1	396.99284
MAL-unique	C16 H15 O8 Br1	412.98776
MAL-unique	C16 H15 O9 Br1	428.98267
MAL-unique	C16 H17 O6 Br1	383.01358
MAL-unique	C16 H17 O7 Br1	399.00849
MAL-unique	C16 H17 O9 Br1	430.99832

MAL-unique	C16 H19 O6 Br1	385.02923
MAL-unique	C16 H19 O9 Br1	433.01397
MAL-unique	C16 H21 O6 Br1	387.04488
MAL-unique	C16 H21 O7 Br1	403.03979
MAL-unique	C17 H13 O10 Br1	454.96194
MAL-unique	C17 H13 O7 Br1	406.97719
MAL-unique	C17 H13 O8 Br1	422.97211
MAL-unique	C17 H13 O9 Br1	438.96702
MAL-unique	C17 H15 O10 Br1	456.97759
MAL-unique	C17 H15 O7 Br1	408.99284
MAL-unique	C17 H15 O8 Br1	424.98776
MAL-unique	C17 H15 O9 Br1	440.98267
MAL-unique	C17 H17 O10 Br1	458.99324
MAL-unique	C17 H17 O6 Br1	395.01358
MAL-unique	C17 H17 O7 Br1	411.00849
MAL-unique	C17 H17 O8 Br1	427.00341
MAL-unique	C17 H17 O9 Br1	442.99832
MAL-unique	C17 H19 O10 Br1	461.00889
MAL-unique	C17 H19 O7 Br1	413.02414
MAL-unique	C17 H19 O8 Br1	429.01906
MAL-unique	C17 H21 O6 Br1	399.04488
MAL-unique	C17 H21 O9 Br1	447.02962
MAL-unique	C18 H13 O8 Br1	434.97211
MAL-unique	C18 H13 O9 Br1	450.96702
MAL-unique	C18 H15 O10 Br1	468.97759
MAL-unique	C18 H15 O7 Br1	420.99284
MAL-unique	C18 H15 O8 Br1	436.98776
MAL-unique	C18 H15 O9 Br1	452.98267
MAL-unique	C18 H17 O10 Br1	470.99324
MAL-unique	C18 H17 O11 Br1	486.98815
MAL-unique	C18 H17 O8 Br1	439.00341
MAL-unique	C18 H17 O9 Br1	454.99832
MAL-unique	C18 H19 O10 Br1	473.00889
MAL-unique	C18 H19 O7 Br1	425.02414
MAL-unique	C18 H19 O8 Br1	441.01906
MAL-unique	C18 H21 O6 Br1	411.04488
MAL-unique	C18 H21 O7 Br1	427.03979
MAL-unique	C18 H21 O8 Br1	443.03471
MAL-unique	C18 H21 O9 Br1	459.02962
MAL-unique	C18 H23 O9 Br1	461.04527
MAL-unique	C19 H15 O10 Br1	480.97759
MAL-unique	C19 H15 O9 Br1	464.98267
MAL-unique	C19 H17 O10 Br1	482.99324
MAL-unique	C19 H17 O7 Br1	435.00849
MAL-unique	C19 H17 O8 Br1	451.00341
MAL-unique	C19 H17 O9 Br1	466.99832

MAL-unique	C19 H19 O10 Br1	485.00889
MAL-unique	C19 H19 O8 Br1	453.01906
MAL-unique	C19 H21 O10 Br1	487.02454
MAL-unique	C19 H21 O7 Br1	439.03979
MAL-unique	C19 H21 O8 Br1	455.03471
MAL-unique	C19 H21 O9 Br1	471.02962
MAL-unique	C19 H23 O6 Br1	425.06053
MAL-unique	C19 H23 O7 Br1	441.05544
MAL-unique	C19 H23 O8 Br1	457.05036
MAL-unique	C19 H23 O9 Br1	473.04527
MAL-unique	C19 H25 O7 Br1	443.07109
MAL-unique	C20 H19 O9 Br1	481.01397
MAL-unique	C20 H21 O10 Br1	499.02454
MAL-unique	C20 H21 O8 Br1	467.03471
MAL-unique	C20 H21 O9 Br1	483.02962
MAL-unique	C20 H23 O9 Br1	485.04527
MAL-unique	C21 H21 O11 Br1	527.01945
MAL-unique	C21 H23 O9 Br1	497.04527
MAL-unique	C27 H23 O5 Cl1	461.11613
MAL-unique	C5 H1 O3 Br3	344.74031
MAL-unique	C7 H7 O5 Br1	248.94041
LIN+NOR	C12 H12 O7 Cl2	336.98874
LIN+NOR	C13 H10 O9 Cl2	378.96292
LIN+NOR	C13 H11 O8 Cl1	329.00697
LIN+NOR	C13 H11 O9 Cl1	345.00189
LIN+NOR	C13 H12 O8 Cl2	364.98365
LIN+NOR	C13 H14 O8 Cl2	366.9993
LIN+NOR	C13 H14 O9 Cl2	382.99422
LIN+NOR	C14 H11 O8 Cl1	341.00697
LIN+NOR	C14 H12 O10 Cl2	408.97348
LIN+NOR	C14 H13 O6 Cl1	311.03279
LIN+NOR	C14 H15 O9 Cl1	361.03319
LIN+NOR	C14 H16 O8 Cl2	381.01495
LIN+NOR	C14 H19 O7 Cl1	333.07466
LIN+NOR	C15 H13 O10 Cl1	387.01245
LIN+NOR	C15 H14 O10 Cl2	422.98913
LIN+NOR	C15 H14 O7 Cl2	375.00439
LIN+NOR	C15 H15 O10 Cl1	389.0281
LIN+NOR	C15 H16 O7 Cl2	377.02004
LIN+NOR	C15 H16 O9 Cl2	409.00987
LIN+NOR	C15 H17 O10 Cl1	391.04375
LIN+NOR	C15 H18 O8 Cl2	395.0306
LIN+NOR	C15 H19 O8 Cl1	361.06957
LIN+NOR	C16 H14 O8 Cl2	402.9993
LIN+NOR	C16 H14 O9 Cl2	418.99422
LIN+NOR	C16 H16 O8 Cl2	405.01495

LIN+NOR	C16 H18 O8 Cl2	407.0306
LIN+NOR	C16 H18 O9 Cl2	423.02552
LIN+NOR	C16 H19 O10 Cl1	405.0594
LIN+NOR	C16 H19 O9 Cl1	389.06449
LIN+NOR	C16 H21 O8 Cl1	375.08522
LIN+NOR	C17 H13 O11 Cl1	427.00737
LIN+NOR	C17 H14 O11 Cl2	462.98405
LIN+NOR	C17 H16 O10 Cl2	449.00478
LIN+NOR	C17 H17 O11 Cl1	431.03867
LIN+NOR	C17 H18 O9 Cl2	435.02552
LIN+NOR	C17 H19 O10 Cl1	417.0594
LIN+NOR	C17 H23 O7 Cl1	373.10596
LIN+NOR	C18 H23 O9 Cl1	417.09579
LIN+NOR	C18 H25 O7 Cl1	387.12161
LIN+NOR	C19 H21 O10 Cl1	443.07505
LIN+NOR	C20 H29 O7 Cl1	415.15291
LIN+STO	C12 H10 O8 Cl2	350.968
LIN+STO	C14 H15 O10 Cl1	377.0281
LIN+STO	C15 H12 O10 Cl2	420.97348
LIN+STO	C16 H11 O9 Cl1	381.00189
LIN+STO	C18 H21 O10 Cl1	431.07505
LIN+STO	C19 H23 O10 Cl1	445.0907
NOR+STO	C12 H12 O9 Cl2	368.97857
NOR+STO	C13 H11 O6 Cl1	297.01714
NOR+STO	C13 H13 O6 Cl1	299.03279
NOR+STO	C13 H13 O8 Cl1	331.02262
NOR+STO	C13 H15 O6 Cl1	301.04844
NOR+STO	C13 H15 O7 Cl1	317.04336
NOR+STO	C13 H16 O7 Cl2	353.02004
NOR+STO	C14 H15 O5 Cl1	297.05353
NOR+STO	C14 H17 O6 Cl1	315.06409
NOR+STO	C15 H11 O8 Cl1	353.00697
NOR+STO	C15 H11 O9 Cl1	369.00189
NOR+STO	C15 H12 O9 Cl2	404.97857
NOR+STO	C15 H13 O7 Cl1	339.02771
NOR+STO	C15 H15 O6 Cl1	325.04844
NOR+STO	C15 H19 O6 Cl1	329.07974
NOR+STO	C15 H28 O3 Cl1 Br1	369.08376
NOR+STO	C15 H30 O3 Cl1 Br1	371.09941
NOR+STO	C16 H15 O7 Cl1	353.04336
NOR+STO	C16 H17 O6 Cl1	339.06409
NOR+STO	C17 H17 O7 Cl1	367.05901
NOR+STO	C17 H21 O8 Cl1	387.08522
NOR+STO	C18 H17 O8 Cl1	395.05392
NOR+STO	C18 H19 O7 Cl1	381.07466
NOR+STO	C19 H19 O9 Cl1	425.06449

NOR+STO	C19 H21 O8 Cl1	411.08522
NOR+STO	C20 H19 O11 Cl1	469.05432
NOR+STO	C20 H23 O9 Cl1	441.09579
NOR+MAL	C16 H19 O7 Br1	401.02414
NOR+MAL	C17 H21 O8 Br1	431.03471
STO+MAL	C13 H11 O7 Br1	356.96154
STO+MAL	C13 H13 O7 Br1	358.97719
STO+MAL	C14 H13 O7 Br1	370.97719
STO+MAL	C15 H13 O8 Br1	398.97211
STO+MAL	C15 H15 O7 Br1	384.99284
STO+MAL	C15 H15 O8 Br1	400.98776
STO+MAL	C15 H17 O6 Br1	371.01358
STO+MAL	C16 H17 O8 Br1	415.00341
STO+MAL	C16 H19 O8 Br1	417.01906
STO+MAL	C17 H19 O9 Br1	445.01397
STO+MAL	C17 H21 O7 Br1	415.03979
STO+MAL	C18 H19 O9 Br1	457.01397
STO+MAL	C18 H23 O7 Br1	429.05544
LIN+NOR+STO	C12 H12 O8 Cl2	352.98365
LIN+NOR+STO	C13 H11 O7 Cl1	313.01206
LIN+NOR+STO	C13 H12 O9 Cl2	380.97857
LIN+NOR+STO	C13 H13 O7 Cl1	315.02771
LIN+NOR+STO	C13 H14 O7 Cl2	351.00439
LIN+NOR+STO	C13 H15 O8 Cl1	333.03827
LIN+NOR+STO	C14 H10 O8 Cl2	374.968
LIN+NOR+STO	C14 H11 O9 Cl1	357.00189
LIN+NOR+STO	C14 H12 O8 Cl2	376.98365
LIN+NOR+STO	C14 H12 O9 Cl2	392.97857
LIN+NOR+STO	C14 H13 O7 Cl1	327.02771
LIN+NOR+STO	C14 H13 O8 Cl1	343.02262
LIN+NOR+STO	C14 H13 O9 Cl1	359.01754
LIN+NOR+STO	C14 H14 O8 Cl2	378.9993
LIN+NOR+STO	C14 H14 O9 Cl2	394.99422
LIN+NOR+STO	C14 H15 O6 Cl1	313.04844
LIN+NOR+STO	C14 H15 O7 Cl1	329.04336
LIN+NOR+STO	C14 H15 O8 Cl1	345.03827
LIN+NOR+STO	C14 H17 O7 Cl1	331.05901
LIN+NOR+STO	C14 H17 O8 Cl1	347.05392
LIN+NOR+STO	C15 H13 O8 Cl1	355.02262
LIN+NOR+STO	C15 H13 O9 Cl1	371.01754
LIN+NOR+STO	C15 H14 O8 Cl2	390.9993
LIN+NOR+STO	C15 H14 O9 Cl2	406.99422
LIN+NOR+STO	C15 H15 O7 Cl1	341.04336
LIN+NOR+STO	C15 H15 O9 Cl1	373.03319
LIN+NOR+STO	C15 H16 O8 Cl2	393.01495
LIN+NOR+STO	C15 H17 O6 Cl1	327.06409

LIN+NOR+STO	C15 H17 O7 Cl1	343.05901
LIN+NOR+STO	C15 H17 O9 Cl1	375.04884
LIN+NOR+STO	C15 H19 O7 Cl1	345.07466
LIN+NOR+STO	C16 H13 O10 Cl1	399.01245
LIN+NOR+STO	C16 H13 O8 Cl1	367.02262
LIN+NOR+STO	C16 H13 O9 Cl1	383.01754
LIN+NOR+STO	C16 H14 O10 Cl2	434.98913
LIN+NOR+STO	C16 H15 O10 Cl1	401.0281
LIN+NOR+STO	C16 H17 O10 Cl1	403.04375
LIN+NOR+STO	C16 H19 O6 Cl1	341.07974
LIN+NOR+STO	C16 H19 O8 Cl1	373.06957
LIN+NOR+STO	C16 H21 O7 Cl1	359.09031
LIN+NOR+STO	C17 H19 O7 Cl1	369.07466
LIN+NOR+STO	C17 H19 O8 Cl1	385.06957
LIN+NOR+STO	C17 H21 O7 Cl1	371.09031
LIN+NOR+STO	C17 H21 O9 Cl1	403.08014
LIN+NOR+STO	C18 H17 O10 Cl1	427.04375
LIN+NOR+STO	C18 H17 O11 Cl1	443.03867
LIN+NOR+STO	C18 H19 O10 Cl1	429.0594
LIN+NOR+STO	C18 H19 O9 Cl1	413.06449
LIN+NOR+STO	C18 H23 O8 Cl1	401.10087
LIN+NOR+STO	C18 H25 O8 Cl1	403.11652
LIN+NOR+STO	C19 H21 O9 Cl1	427.08014
LIN+NOR+STO	C19 H23 O9 Cl1	429.09579
LIN+NOR+MAL	C17 H17 O10 Cl1	415.04375
LIN+STO+MAL	C5 H1 O3 Cl1 Br2	300.79082
NOR+STO+MAL	C18 H23 O8 Br1	445.05036
LIN+NOR+STO+MAL	C15 H15 O8 Cl1	357.03827
LIN+NOR+STO+MAL	C15 H17 O8 Cl1	359.05392
LIN+NOR+STO+MAL	C16 H15 O8 Cl1	369.03827
LIN+NOR+STO+MAL	C16 H15 O9 Cl1	385.03319
LIN+NOR+STO+MAL	C16 H17 O7 Cl1	355.05901
LIN+NOR+STO+MAL	C16 H17 O8 Cl1	371.05392
LIN+NOR+STO+MAL	C16 H17 O9 Cl1	387.04884
LIN+NOR+STO+MAL	C16 H19 O7 Cl1	357.07466
LIN+NOR+STO+MAL	C17 H15 O9 Cl1	397.03319
LIN+NOR+STO+MAL	C17 H17 O8 Cl1	383.05392
LIN+NOR+STO+MAL	C17 H17 O9 Cl1	399.04884
LIN+NOR+STO+MAL	C17 H19 O9 Cl1	401.06449
LIN+NOR+STO+MAL	C18 H19 O8 Cl1	397.06957
LIN+NOR+STO+MAL	C18 H21 O7 Cl1	383.09031
LIN+NOR+STO+MAL	C18 H21 O8 Cl1	399.08522
LIN+NOR+STO+MAL	C18 H21 O9 Cl1	415.08014

Table S3 Comparison with previous non-target studies on DBPs formed in drinking water treatment.

Study	Lavonen 2013	Lavonen 2013	Lavonen 2013	Lavonen 2013	Gonsior 2014	Zhang 2012b
WTP	Lovö	Lackarebäck	Kvarnagården	Ringsjö	Råberga	Mopanshan
Country	Sweden	Sweden	Sweden	Sweden	Sweden	China
Water source	Lake Mälaren	Delsjö lakes	Lake Neden + 1/4 groundwater	Lake Bolmen + 1/8 groundwater	Stångån River	Mopanshan reservoir
Disinfectant	NH ₂ Cl	ClO ₂ + Cl ₂	NH ₂ Cl	NaOCl	NaOCl	NaOCl
Dose (mg/L as Cl ₂)	0.27	0.39 + 0.86	0.3	0.88	0.36	1.8
SPE cartridge	Bond Elut PPL	Bond Elut PPL	Bond Elut PPL	Bond Elut PPL	Bond Elut PPL	Sep-pak C18
Variable compared	Neutral Formula	Neutral Formula	Neutral Formula	Neutral Formula	Theoretical Mass Neg. Ion	Theoretical Mass Neg. Ion
Number of DBPs matching	12	32	15	73	84	28
% of DBPs matching (of the 360 individual formulae detected in this study)	3%	9%	4%	20%	23%	8%

Table S4 Comparison with previous non-target studies on DBPs formed in formation potential experiments.

Study	Zhang 2012a	Zhang 2014	Zhang 2018
NOM source	Taihe, huangpujiang and Miyun	Suwannee River fulvic acid	Suwannee River fulvic acid
Disinfectant	NaOCl	NaOCl	NH ₂ Cl
Dose (mg/L as Cl ₂)	20	5	5
Addition of NaBr (mg/L)	-	2	2
pH	7.2	7.5	7.5
Reaction time (days)	7	5	5
SPE cartridge	Sep-pak C18	Sep-pak C18	Sep-pak C18
Variable compared	Theoretical Mass Neg. Ion	Theoretical Mass Neg. Ion	Theoretical Mass Neg. Ion
Number of DBPs matching	225	334	63
% of DBPs matching (of the 360 individual formulae detected in this study)	63%	93%	18% (49 % if only Br-DBPs compared)

Table S5 Comparison with a previous non-target study on DBPs formed in a formation potential experiment on separated NOM fractions.

Study	Harris 2015	Harris 2015	Harris 2015	Harris 2015	Harris 2015
NOM source	Suwannee River fulvic acid	Suwannee River fulvic acid	Suwannee River fulvic acid	Suwannee River fulvic acid	Suwannee River fulvic acid
NOM fractionation	X-Bridge phenyl column	X-Bridge phenyl column	X-Bridge phenyl column	X-Bridge phenyl column	X-Bridge phenyl column
NOM fraction	1	7	30	50	65
NOM fraction description	early- eluting	early- eluting	mid- eluting	late- eluting	late- eluting
NOM fraction characteristics	High O/C, Low H/C	High O/C, Low H/C	Mid O/C, Mid H/C	Low O/C, High H/C	Low O/C, High H/C
Disinfectant	NaOCl	NaOCl	NaOCl	NaOCl	NaOCl
Dose (g/g total Cl ₂ to total organic C)	0.2 ± 0.1	0.2 ± 0.1	0.2 ± 0.1	0.2 ± 0.1	0.2 ± 0.1
pH	4.8 ± 0.9	4.8 ± 0.9	4.8 ± 0.9	4.8 ± 0.9	4.8 ± 0.9
Reaction time (days)	3	3	3	3	3
Variable compared	Neutral Formula	Neutral Formula	Neutral Formula	Neutral Formula	Neutral Formula
Number of DBPs matching	0	37	0	3	28
% of DBPs matching (of the 360 individual formulae detected in this study)	0%	10%	0%	1%	8%