Electronic supplementary information

# Molecular level seasonality of dissolved organic matter in freshwater and its impact on drinking water treatment

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**Figure S1.** Map showing the locations of the cities Linköping (LIN), Norrköping (NOR), Stockholm (STO) and Malmö (MAL), where samples were collected at DWTPs for the study.

**EEM PARAFAC analysis**

PARAFAC modelling of the about 300 EEM spectra resulted in a model explained by five components (Figure S2), which were matched with model components of previous studies (Table 2). In general, fluorescence peaks that emits at high wavelengths, contain many conjugated molecules and components 1, 2, 3 and 4 (C1, C2, C3, C4) have been described as humic-like components and component 5 (C5) as a protein-like component (Fellman et al., 2010). C1 and C2 were the EEM profiles that had the highest count of matches with prior model components (Table 2). C1 has been attributed as terrestrial humic-like material (Fellman et al., 2010, Coble, 1996, Guéguen et al., 2014), and this fluorescent signal has been observed for waters influenced by agriculture (Osburn et al., 2012). C2 has been described as a broader group of both humic-like and fulvic-like components (fulvic acids are typically smaller than humic acids and have a higher oxygen content) (Osburn et al., 2012). Due to the high emission maxima of C3 ( >440 nm, Table 2), this component have been associated with a humic-like component of terrestrial origin (Yang et al., 2015). The fluorescent signal of C4 has shorter emission wavelengths (Table 2), indicating less aromatic character, compared to C1-C3, and has been associated with low molecular weight molecules from other types of sources, e.g., from biological activity (e.g., plankton), in marine environments, and *in situ* production, e.g., primary production of DOM by algae (Fellman et al., 2010, Guéguen et al., 2014, Kellerman et al., 2015).

The fluorescent signal of C5 has been associated with protein-like or tryptophan-like compounds (Coble, 1996, Fellman et al., 2010, Osburn et al., 2012). Tryptophan is an amino acid that carries intrinsic fluorescent properties due to its fused aromatic ring side group; fluorescence from proteins mainly arises from the excitation and emission of the tryptophan side group. The origin of protein-like fluorescence has been linked to microbial activity, e.g., when certain microorganisms release enzymes to break down dead plant material (Wong and Williams, 2010). Protein-like fluorescence has also been found to increase by influences of waste water effluents or during algal blooms (Yang et al., 2015). Through combined fluorescence measurements and liquid chromatography with organic carbon detection (LC-OCD), protein-like fluorescence has been linked to a DOM fraction categorized as the biopolymer fraction (Baghoth et al., 2011).

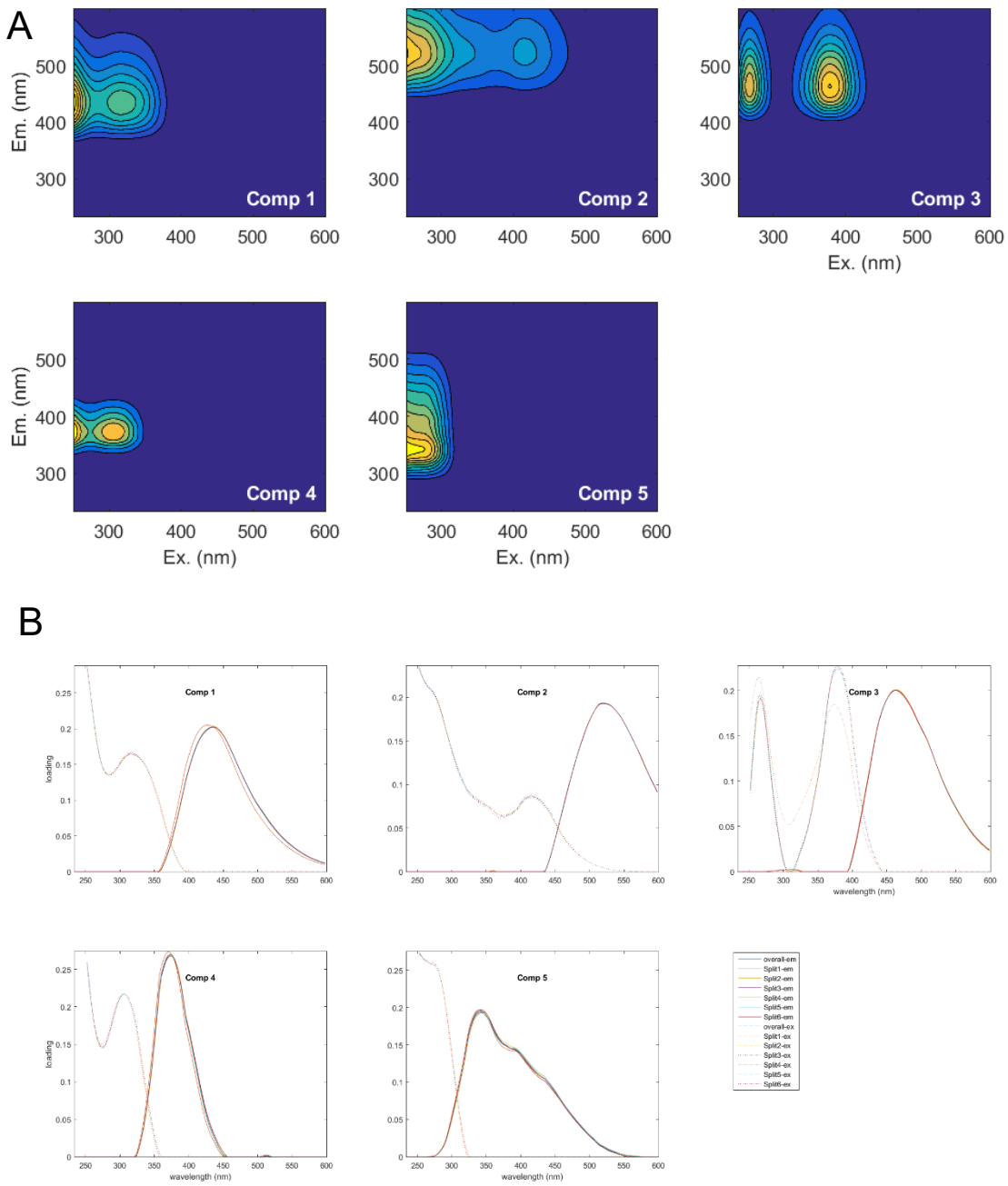


**Figure S2.** EEM spectra of the five components (comp) identified using Parallel Factor Analysis (PARAFAC) (**A**) and excitation/emission spectra of each component during split-validation (**B**).

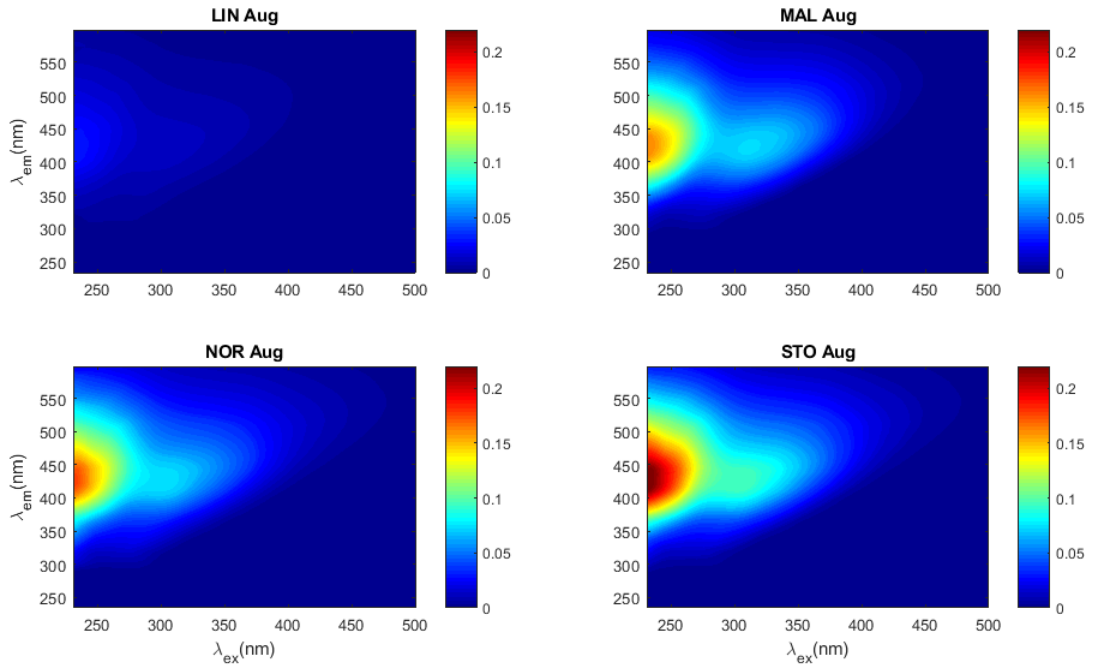


**Figure S3.** Variations in raw water EEM fluorescence spectra compared at the highest fluorescence scale (in Raman units) shown for samples from the four DWTPs collected in August.

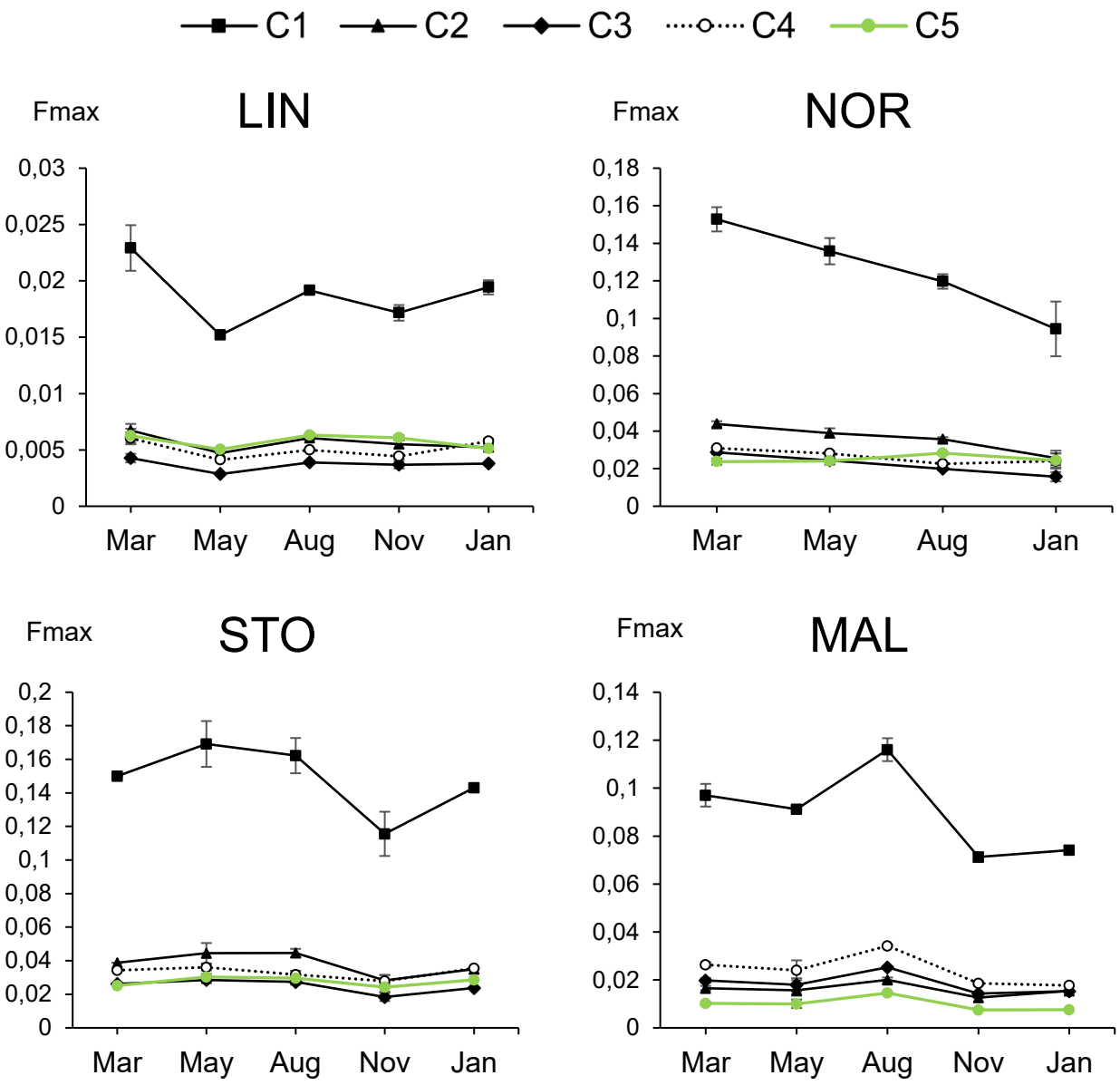


**Figure S4.** Variability in raw water characteristics defined by the five PARAFAC components, C1-C5 (Fig S1). Average values of two replicates and standard deviations are presented. Data for NOR in November is missing. Note the different y-axis scales.

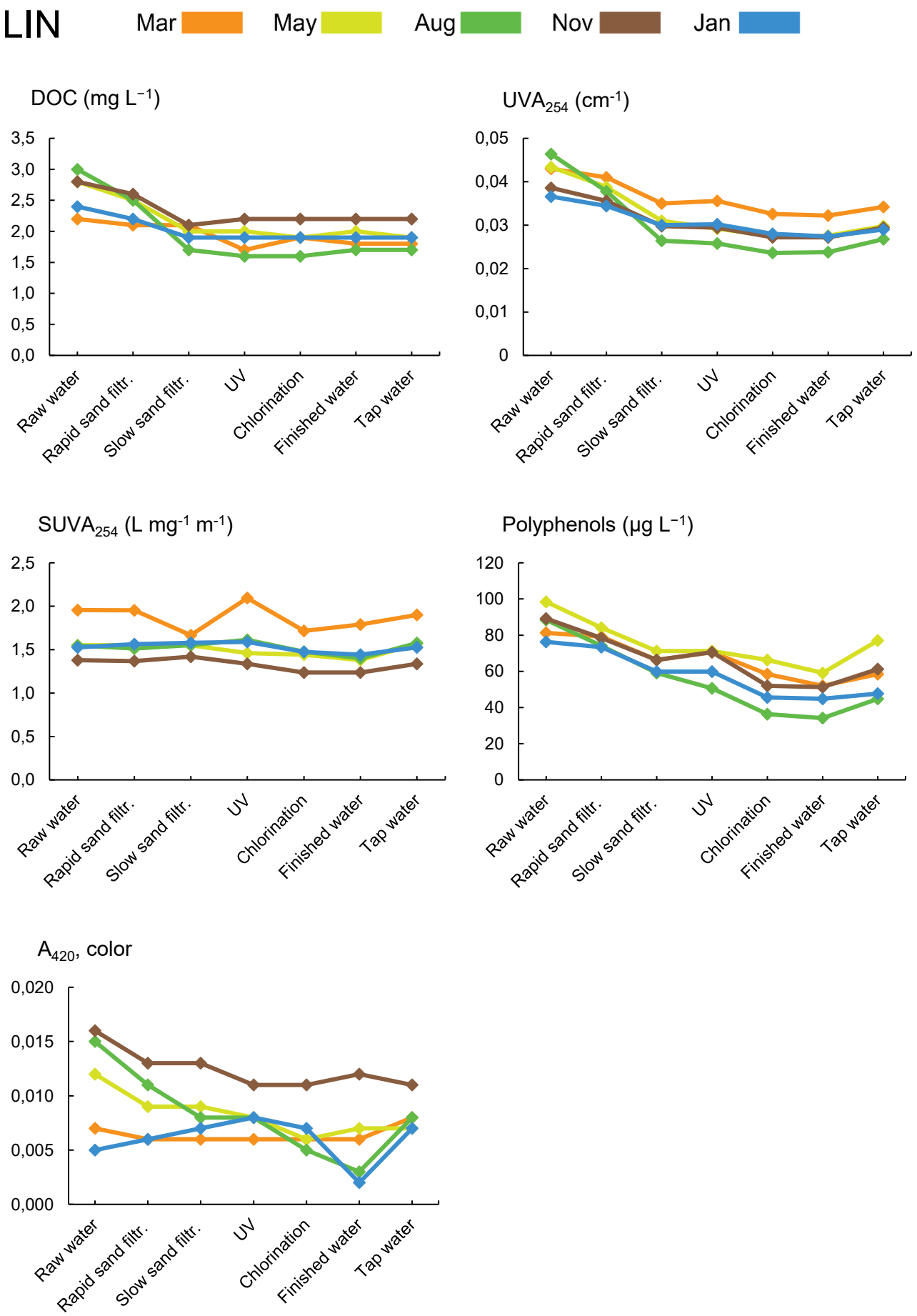


**Figure S5.** Changes in DOC, $UVA_{254}$, $SUVA_{254}$, polyphenols and $A_{420}$ upon treatment at LIN.

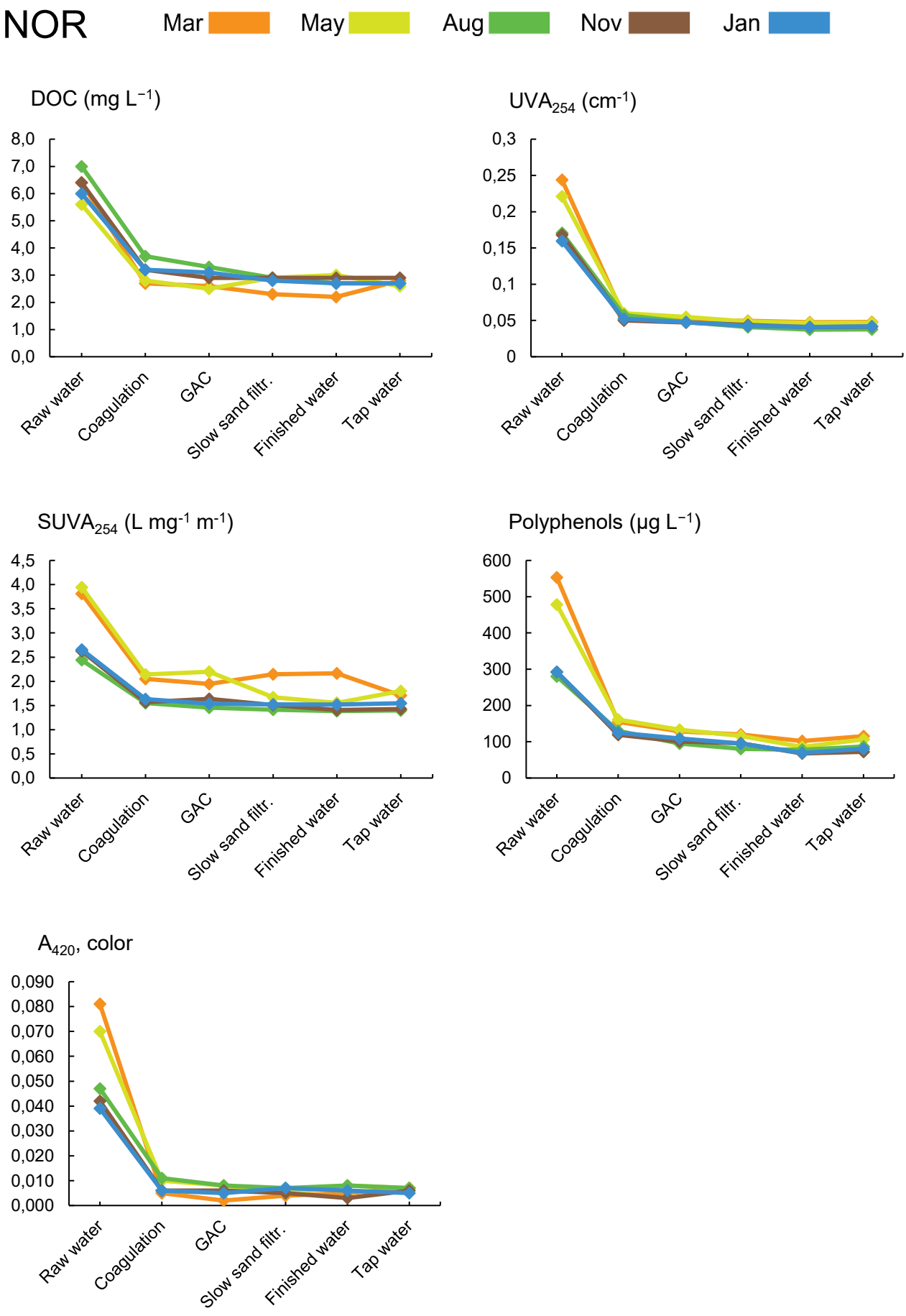


**Figure S6.** Changes in DOC, $UVA_{254}$, $SUVA_{254}$, polyphenols and $A_{420}$ upon treatment at NOR.

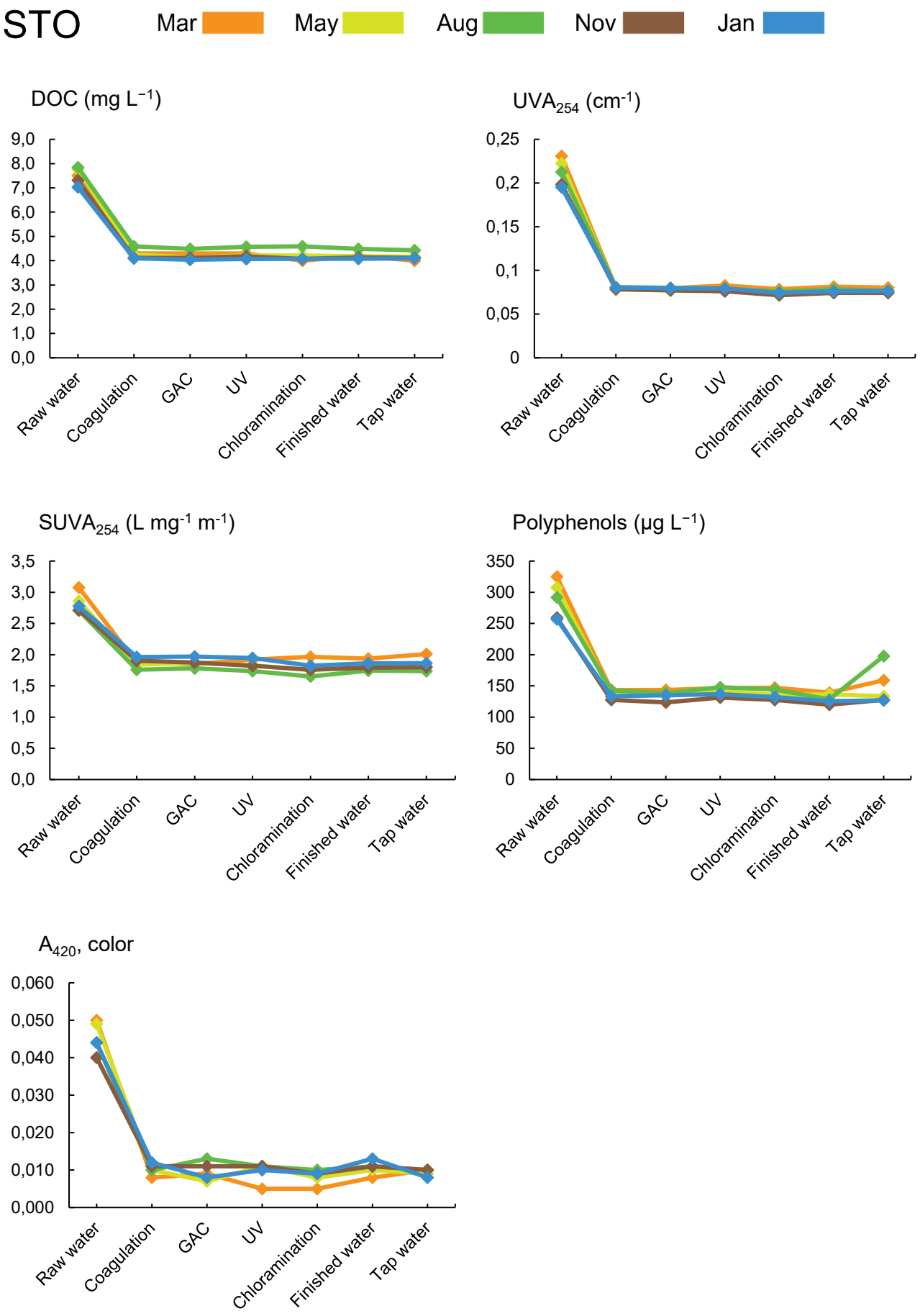


**Figure S7.** Changes in DOC, $UVA_{254}$, $SUVA_{254}$, polyphenols and $A_{420}$ upon treatment at STO.

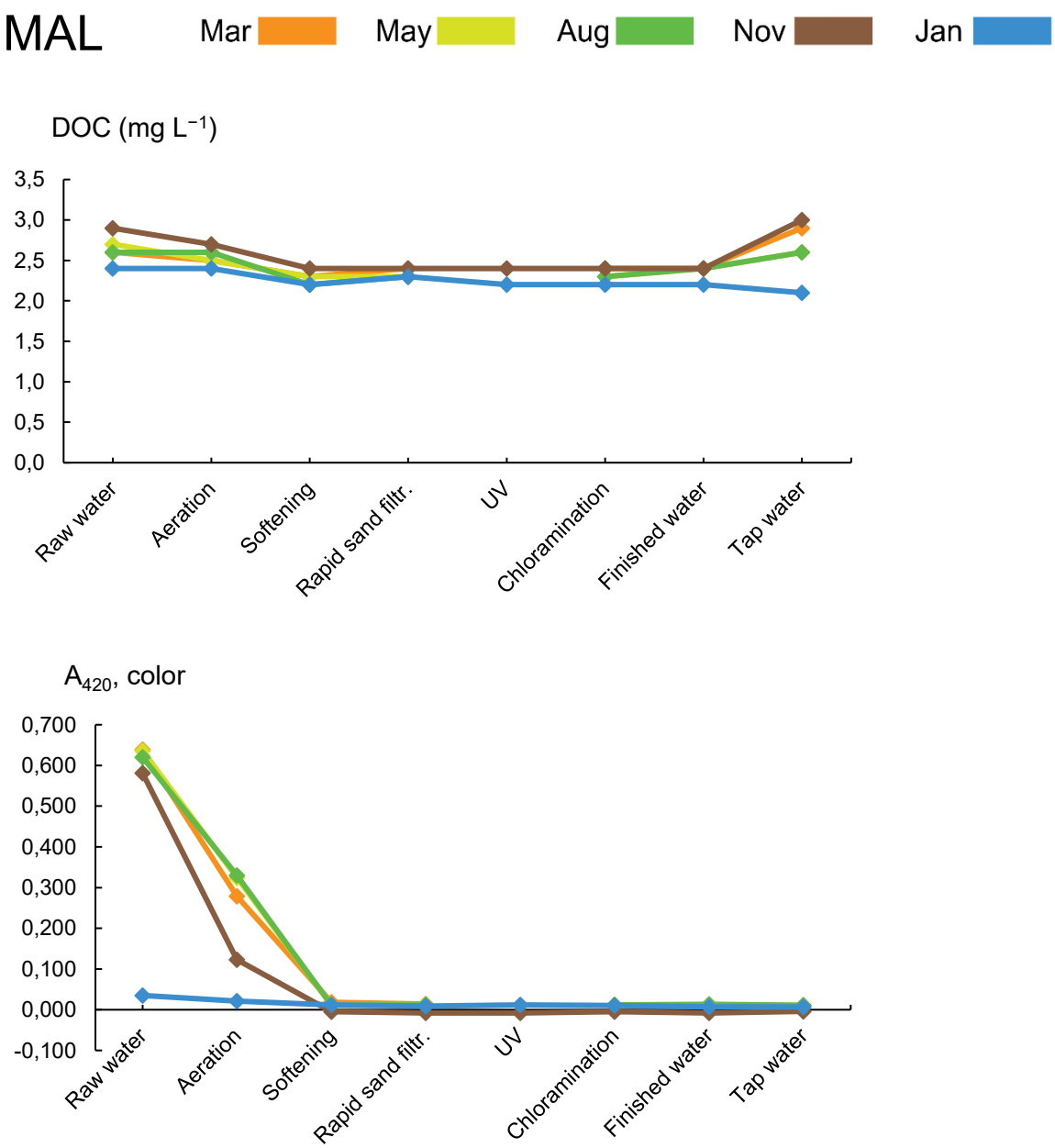


**Figure S8.** Changes in DOC and $A_{420}$ upon treatment at MAL. Data for $UVA_{254}$, $SUVA_{254}$, and polyphenols are not shown due to interferences of iron on absorbance measurements for DOM analysis at this water source. UV was installed during the sample campaign, why data at this sampling point only are available for two occasions.

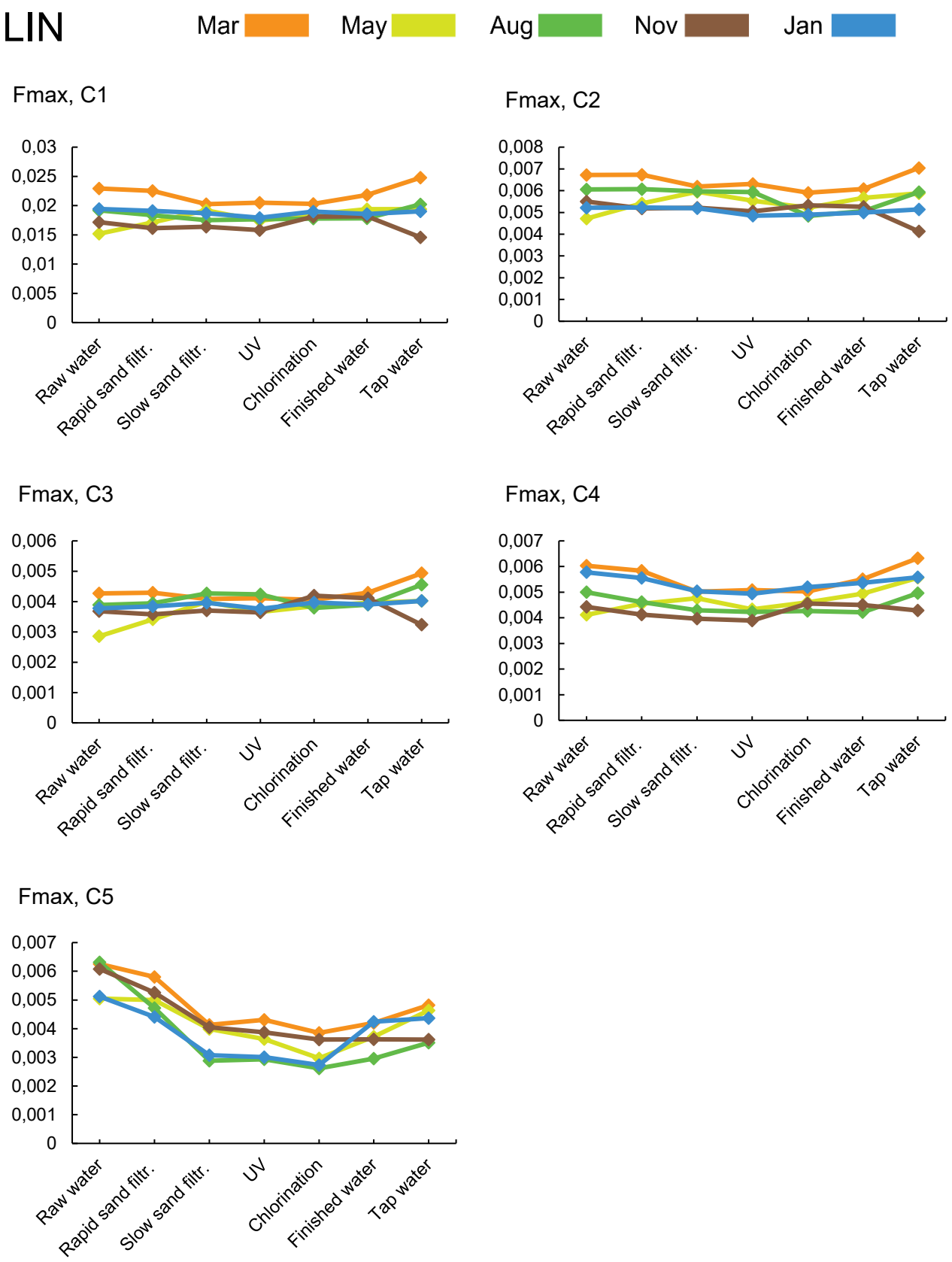


**Figure S9.** Average Fmax values of the five PARAFAC components and the effect of treatment in LIN. The average of two replicates are shown, standard deviations are reported in Table S5.

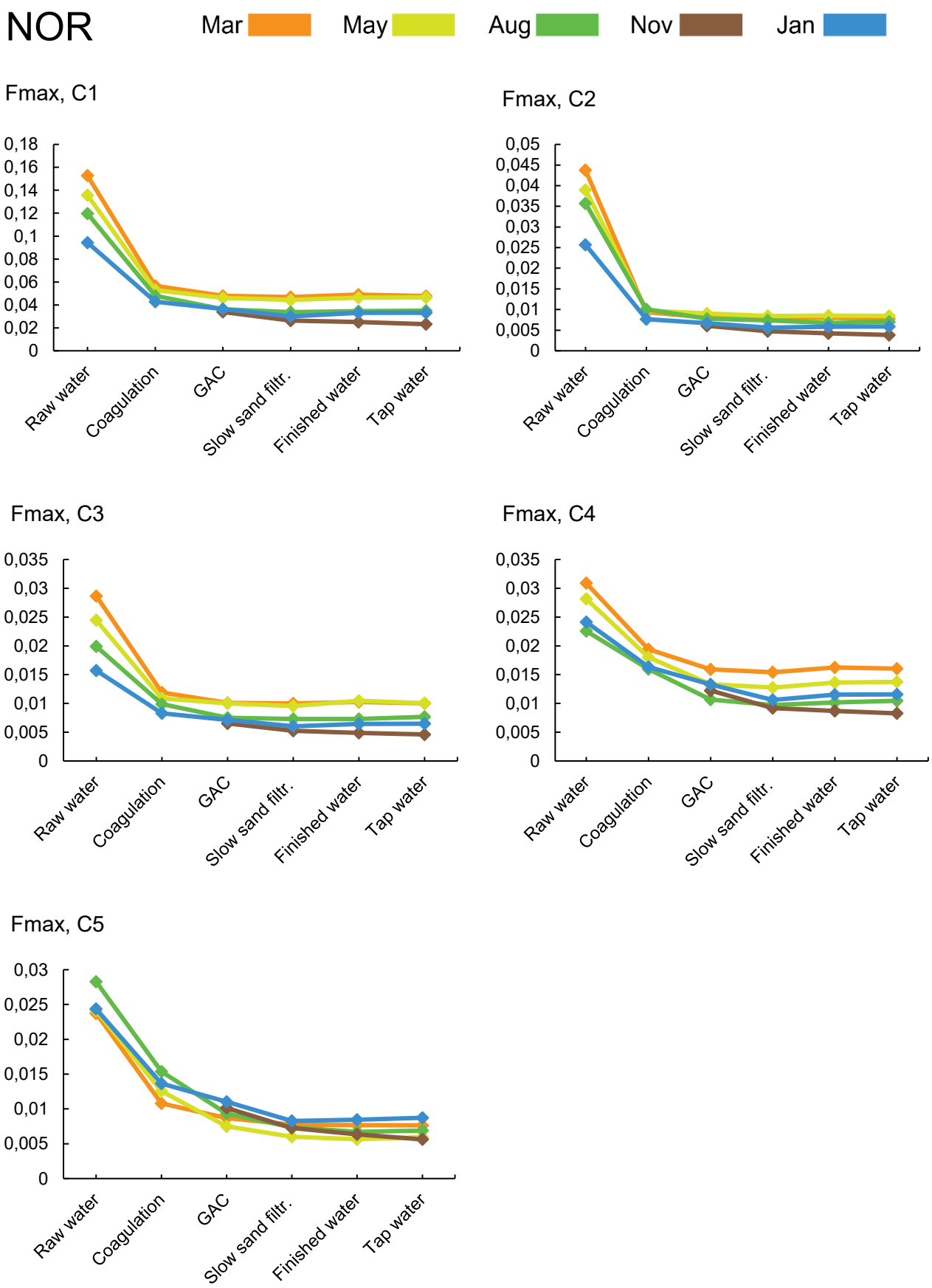


**Figure S10.** Average Fmax values of the five PARAFAC components and the effect of treatment in NOR. The average of two replicates are shown, standard deviations are reported in Table S5. Data for Raw water and coagulation are missing for November.

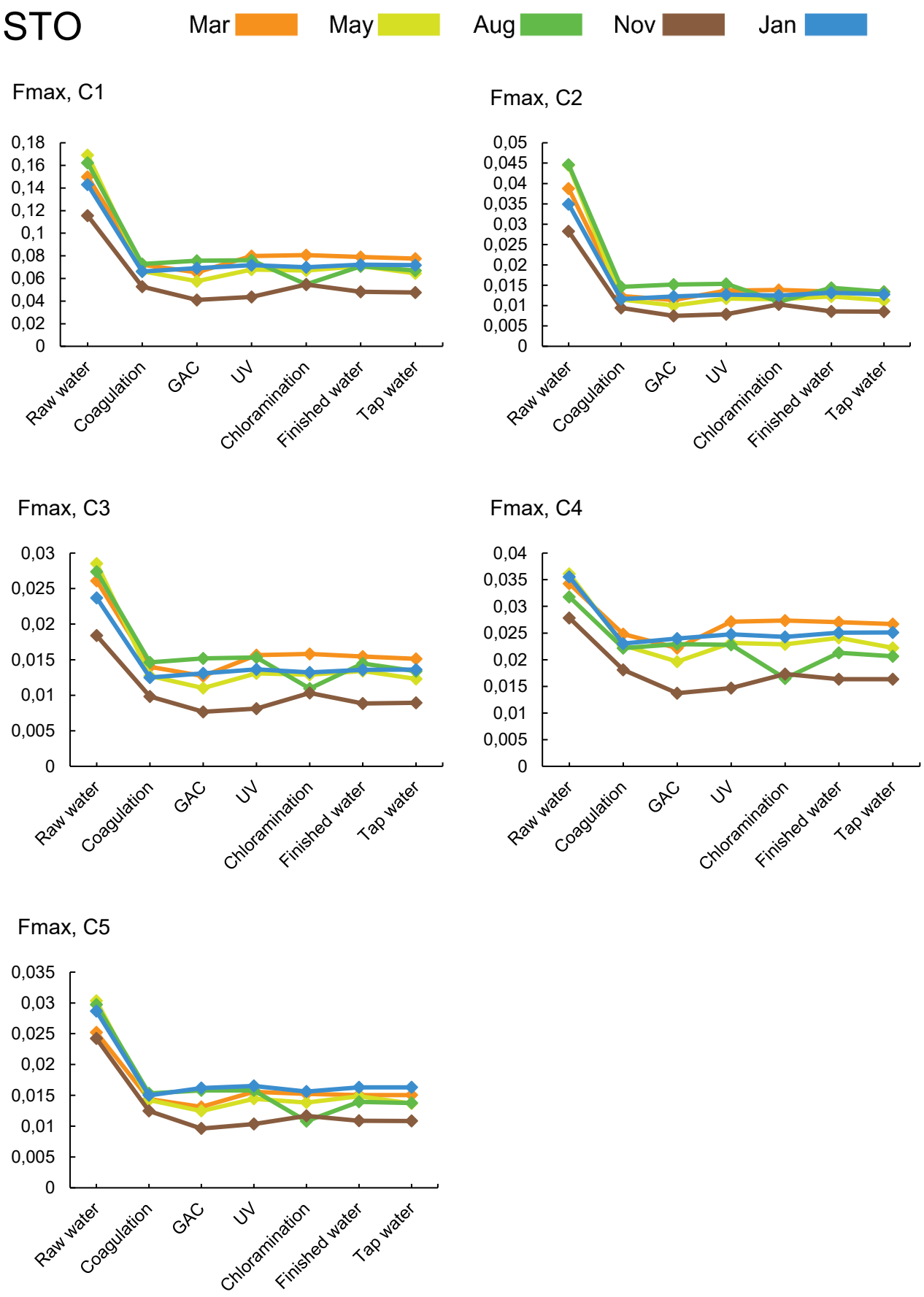


**Figure S11.** Average Fmax values of the five PARAFAC components and the effect of treatment in STO. The average of two replicates are shown, standard deviations are reported in Table S5.

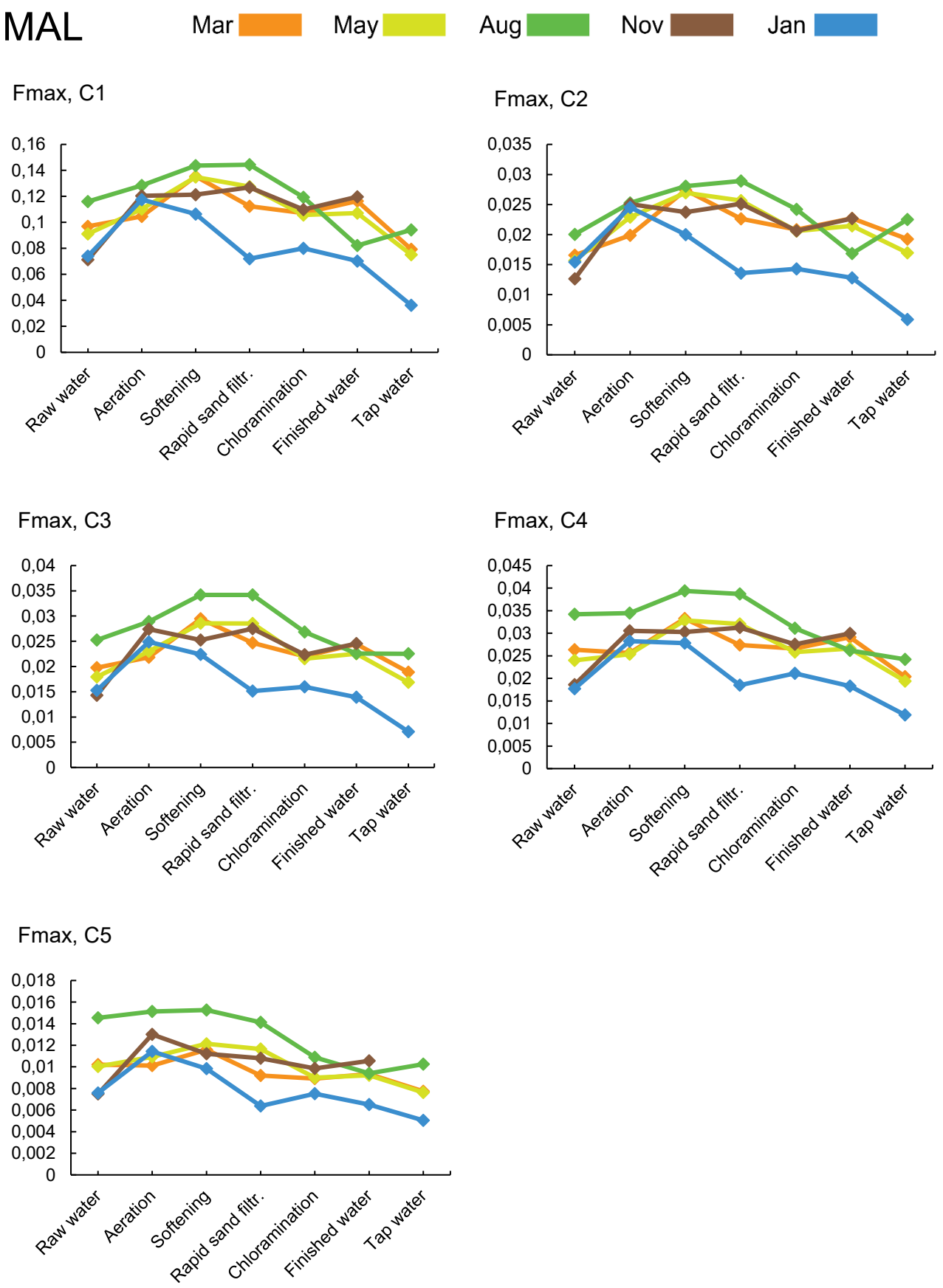


**Figure S12.** Average Fmax values of the five PARAFAC components and the effect of treatment in MAL. The average of two replicates are shown, standard deviations are reported in Table S5.

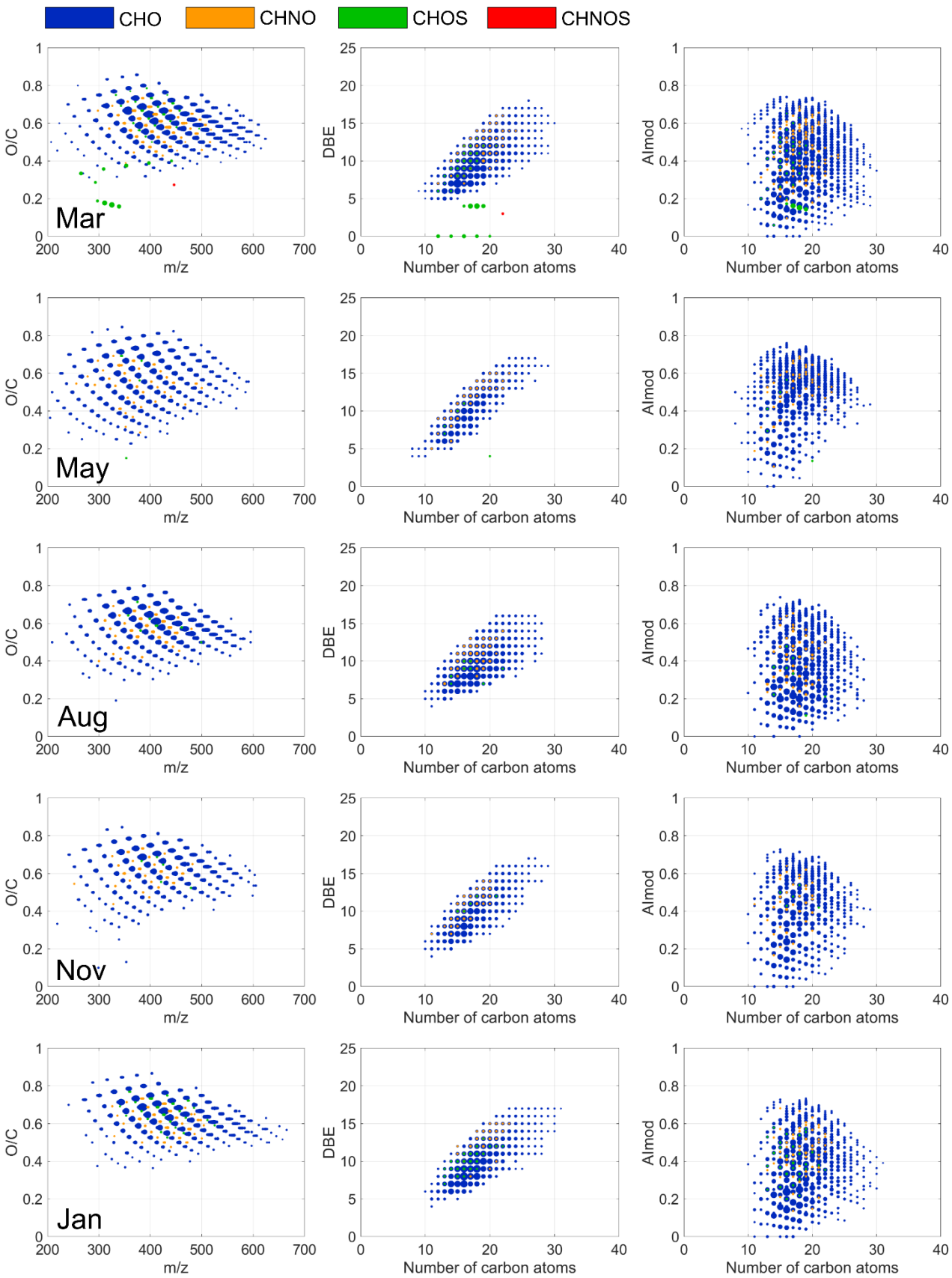


**Figure S13.** Molecular compositions that decreased in relative abundance by more than 50% after coagulation at NOR, presented with mass-edited O/C ratios (left panel), double bond equivalents (DBE) (middle panel) and a modified aromaticity index ($AI_{mod}$) (right panel). DOM changes for five months shown separately. Point size reflect relative mass peak intensity in a sample.

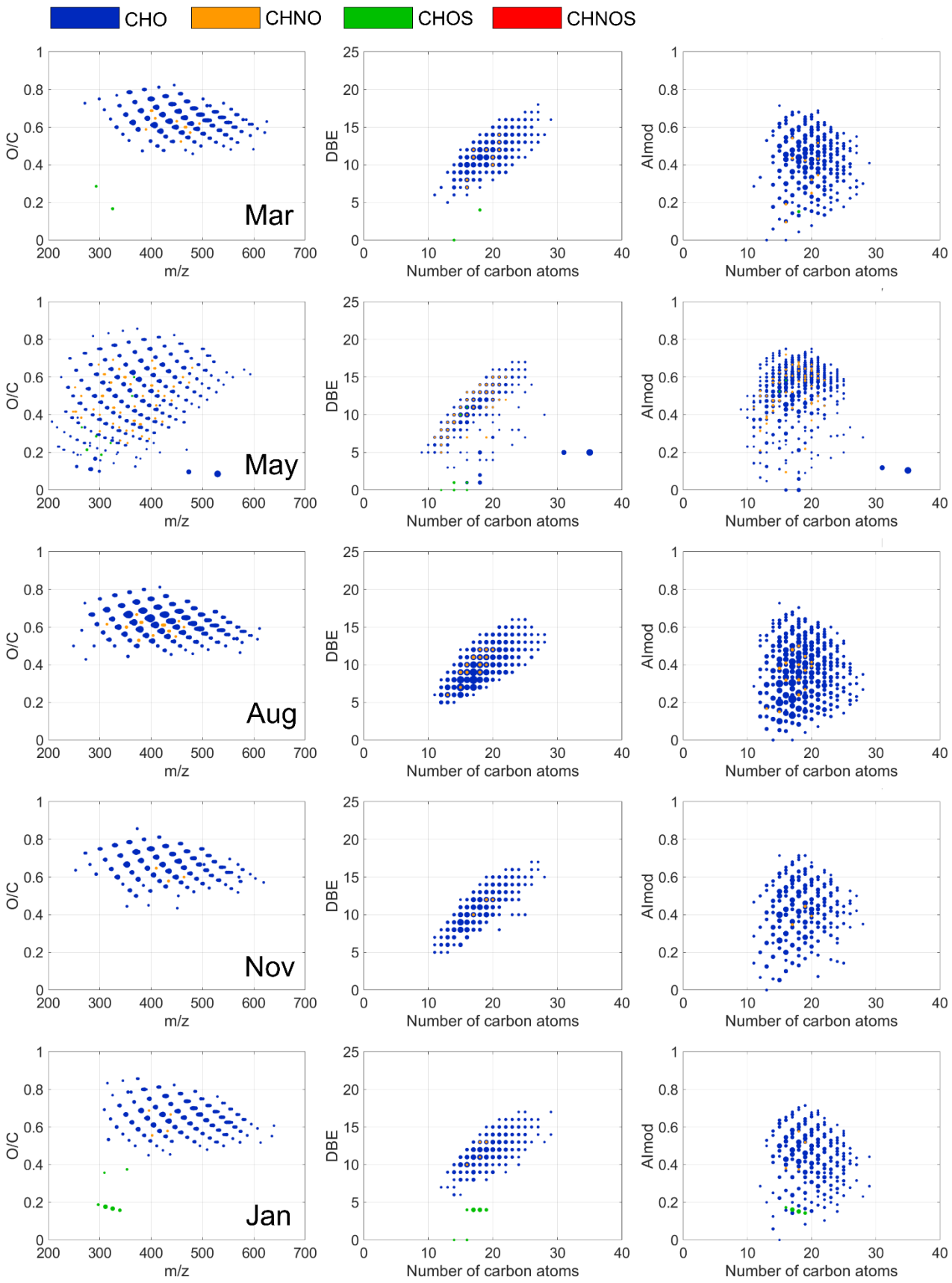


**Figure S14.** Molecular compositions that decreased in relative abundance by more than 50% after coagulation at STO, presented with mass-edited O/C ratios (left panel), double bond equivalents (DBE) (middle panel) and a modified aromaticity index ($AI_{mod}$) (right panel). DOM changes for five months shown separately. Point size reflect relative mass peak intensity in a sample.

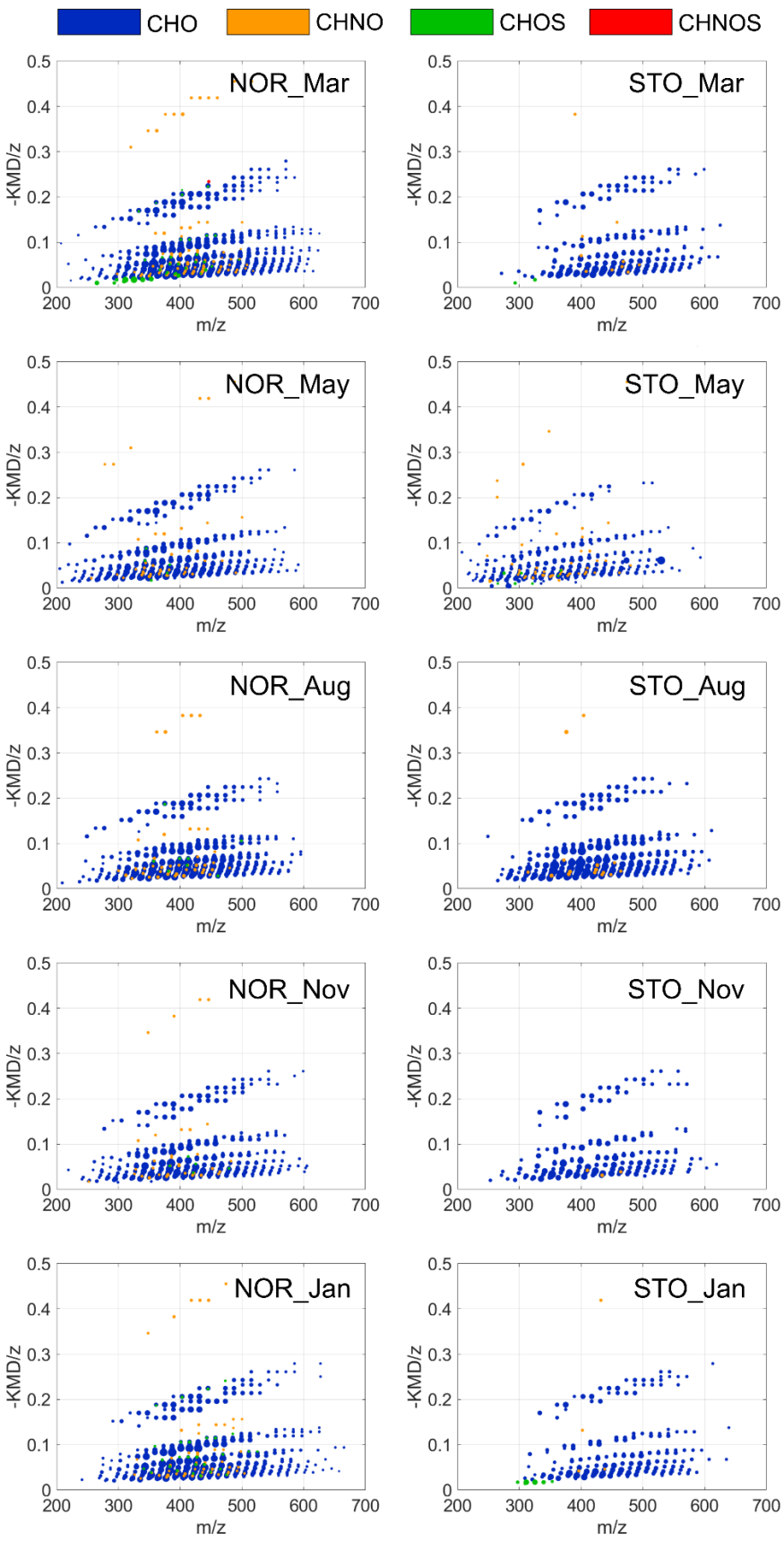


**Figure S15.** Molecular compositions that decreased in relative abundance by more than 50% after coagulation, presented with modified Kendrick mass plots for NOR (left panel) and STO (right panel). DOM changes for five months shown separately. Point size reflect relative mass peak intensity in a sample.

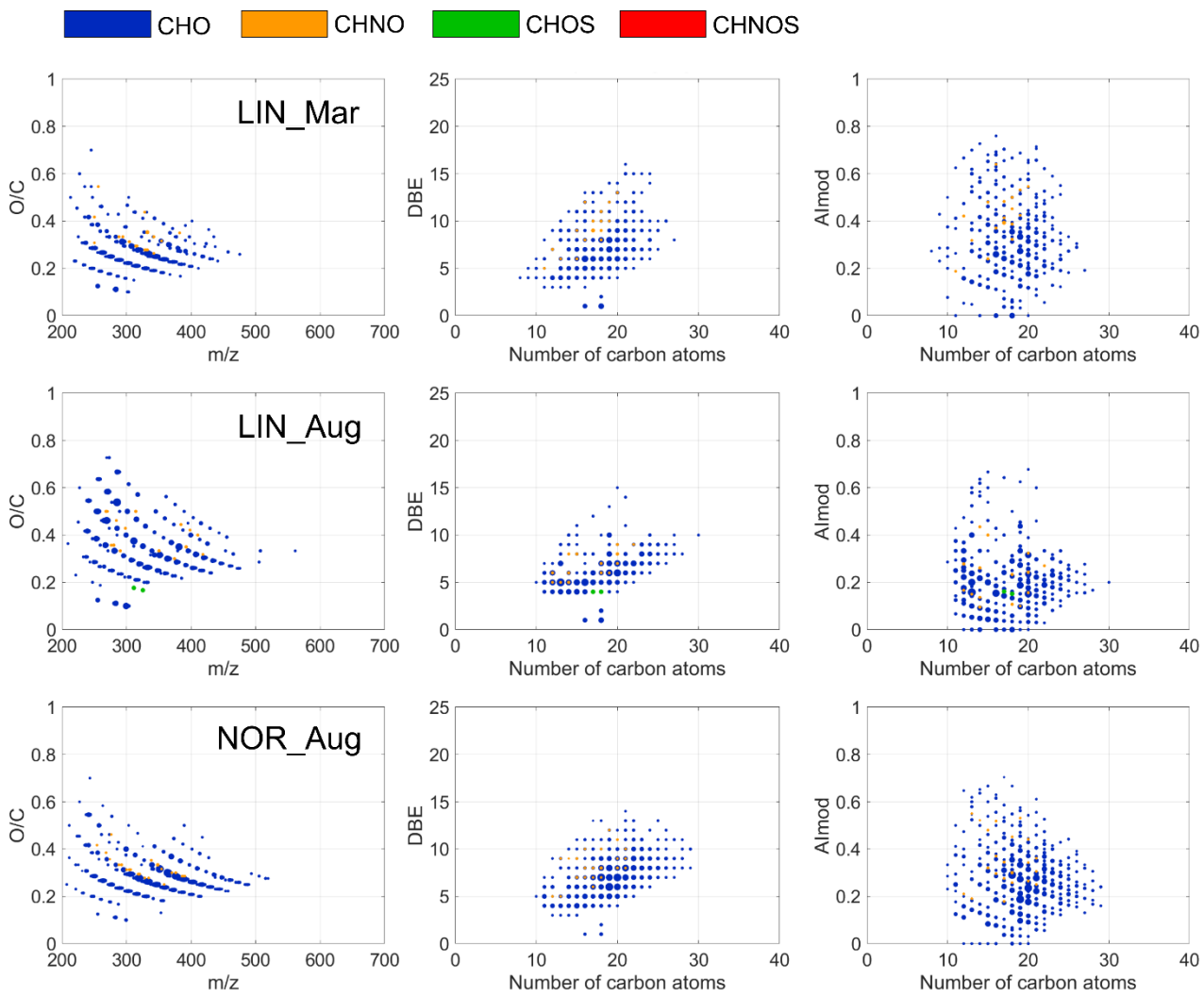


**Figure S16.** Molecular compositions that decreased in relative abundance by more than 50% after slow sand filtration at LIN (March and August) and NOR (August), presented with mass-edited O/C ratios (left panel), double bond equivalents (DBE) (middle panel) and a modified aromaticity index ($AI_{mod}$) (right panel). Point size reflect relative mass peak intensity in a sample.

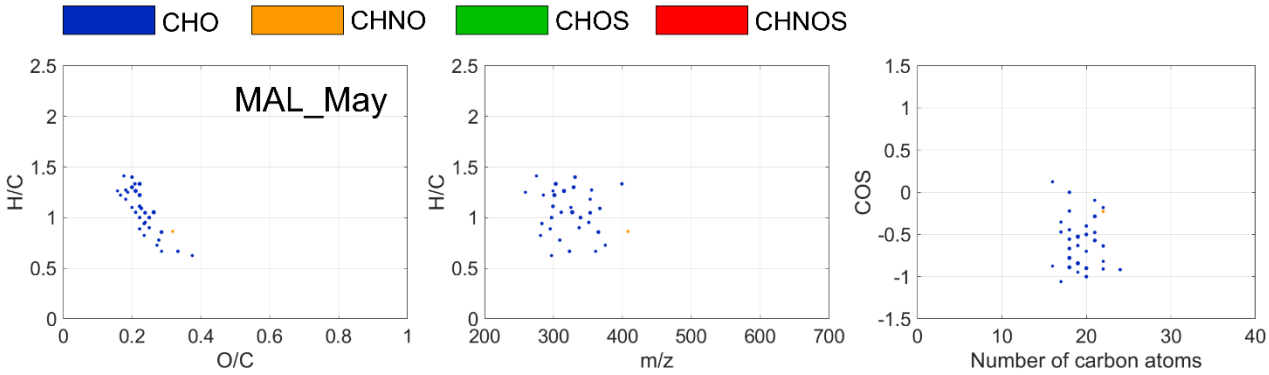


**Figure S17.** Van Krevelen diagrams (left panel), mass edited H/C ratios (middle panel) and average oxidation state of carbon plots (right panel) of the molecular compositions that decreased in relative abundance by more than 50% after softening in MAL in May. Point size reflect relative mass peak intensity in a sample.

**Table S1.** Counts of *m/z* ions and computed indices of molecular formulae detected in the source water of LIN throughout five sample occasions as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added). RSD = relative standard deviation. DBE = Double bond equivalences, $AI_{mod}$ = a modified aromaticity index.

| Characterization of LIN DOM | Mar | May | Aug | Nov | Jan | RSD |
|---|---|---|---|---|---|---|
| number of DOM compositions | 2173 | 2243 | 2076 | 2080 | 1826 | 8% |
| average H [%] | 44.9 | 44.6 | 45.2 | 44.8 | 46.0 | 1% |
| average C [%] | 37.1 | 36.9 | 36.7 | 36.7 | 36.5 | 1% |
| average O [%] | 17.8 | 18.3 | 17.9 | 18.3 | 17.3 | 2% |
| average N [%] | 0.15 | 0.14 | 0.15 | 0.15 | 0.13 | 6% |
| average S [%] | 0.04 | 0.05 | 0.04 | 0.05 | 0.04 | 12% |
| computed average H/C ratio | 1.21 | 1.21 | 1.23 | 1.22 | 1.26 | 2% |
| computed average O/C ratio | 0.48 | 0.50 | 0.49 | 0.50 | 0.47 | 3% |
| computed average N/C ratio | 0.004 | 0.004 | 0.004 | 0.004 | 0.004 | 0% |
| computed average S/C ratio | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0% |
| average carbon oxidation state ($C_{OS}$) | -0.238 | -0.204 | -0.241 | -0.211 | -0.295 | 15% |
| average DBE | 8.2 | 8.3 | 8.0 | 8.1 | 7.9 | 2% |
| average DBE/C | 0.45 | 0.45 | 0.44 | 0.45 | 0.43 | 2% |
| average $AI_{mod}$ | 0.28 | 0.27 | 0.26 | 0.26 | 0.24 | 6% |
| mass weighted average [Da] | 382.3 | 389.6 | 386.2 | 383.9 | 390.4 | 1% |

**Table S2.** Counts of *m/z* ions and computed indices of molecular formulae detected in the source water of NOR throughout five sample occasions as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added). RSD = relative standard deviation. DBE = Double bond equivalences, $AI_{mod}$ = a modified aromaticity index.

| Characterization of NOR DOM | Mar | May | Aug | Nov | Jan | RSD |
|---|---|---|---|---|---|---|
| number of DOM compositions | 2846 | 2388 | 2187 | 2362 | 2859 | 12% |
| average H [%] | 42.9 | 43.8 | 44.4 | 43.5 | 42.7 | 2% |
| average C [%] | 37.8 | 38.1 | 37.7 | 37.4 | 37.4 | 1% |
| average O [%] | 19.0 | 18.0 | 17.7 | 18.9 | 19.6 | 4% |
| average N [%] | 0.14 | 0.14 | 0.13 | 0.14 | 0.14 | 3% |
| average S [%] | 0.09 | 0.05 | 0.05 | 0.07 | 0.11 | 35% |
| computed average H/C ratio | 1.14 | 1.15 | 1.18 | 1.16 | 1.14 | 1% |
| computed average O/C ratio | 0.50 | 0.47 | 0.47 | 0.50 | 0.52 | 4% |
| computed average N/C ratio | 0.004 | 0.004 | 0.004 | 0.004 | 0.004 | 0% |
| computed average S/C ratio | 0.002 | 0.001 | 0.001 | 0.002 | 0.003 | 46% |
| average carbon oxidation state ($C_{OS}$) | -0.117 | -0.189 | -0.222 | -0.139 | -0.083 | 37% |
| average DBE | 9.1 | 8.9 | 8.7 | 8.8 | 9.1 | 2% |
| average DBE/C | 0.49 | 0.48 | 0.47 | 0.47 | 0.48 | 2% |
| average $AI_{mod}$ | 0.31 | 0.32 | 0.30 | 0.29 | 0.29 | 4% |
| mass weighted average [Da] | 399.8 | 385.9 | 388.3 | 396.4 | 407.2 | 2% |

**Table S3.** Counts of *m/z* ions and computed indices of molecular formulae detected in the source water of STO throughout five sample occasions as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added). RSD = relative standard deviation. DBE = Double bond equivalences, $AI_{mod}$ = a modified aromaticity index.

| Characterization of STO DOM | Mar | May | Aug | Nov | Jan | RSD |
|---|---|---|---|---|---|---|
| number of DOM compositions | 2185 | 2719 | 1688 | 1589 | 2198 | 22% |
| average H [%] | 42.9 | 44.7 | 43.5 | 43.1 | 43.0 | 2% |
| average C [%] | 37.4 | 37.7 | 37.3 | 37.3 | 37.3 | 0% |
| average O [%] | 19.5 | 17.4 | 19.0 | 19.4 | 19.5 | 5% |
| average N [%] | 0.11 | 0.15 | 0.10 | 0.09 | 0.10 | 21% |
| average S [%] | 0.08 | 0.05 | 0.05 | 0.05 | 0.09 | 30% |
| computed average H/C ratio | 1.15 | 1.18 | 1.16 | 1.16 | 1.15 | 1% |
| computed average O/C ratio | 0.52 | 0.46 | 0.51 | 0.52 | 0.52 | 5% |
| computed average N/C ratio | 0.003 | 0.004 | 0.003 | 0.003 | 0.003 | 14% |
| computed average S/C ratio | 0.002 | 0.001 | 0.001 | 0.001 | 0.003 | 56% |
| average carbon oxidation state ($C_{OS}$) | -0.095 | -0.245 | -0.133 | -0.106 | -0.098 | 47% |
| average DBE | 9.3 | 8.8 | 9.0 | 8.9 | 9.1 | 2% |
| average DBE/C | 0.48 | 0.46 | 0.47 | 0.48 | 0.48 | 2% |
| average $AI_{mod}$ | 0.29 | 0.30 | 0.29 | 0.29 | 0.29 | 2% |
| mass weighted average [Da] | 417.3 | 392.5 | 407.8 | 404.2 | 414.1 | 2% |

**Table S4.** Counts of *m/z* ions and computed indices of molecular formulae detected in the source water of MAL throughout five sample occasions as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added). RSD = relative standard deviation. DBE = Double bond equivalences, $AI_{mod}$ = a modified aromaticity index.

| Characterization of MAL DOM | Mar | May | Aug | Nov | Jan | RSD |
|---|---|---|---|---|---|---|
| number of DOM compositions | 2062 | 2106 | 2108 | 1927 | 2318 | 7% |
| average H [%] | 44.4 | 44.7 | 44.7 | 44.3 | 44.0 | 1% |
| average C [%] | 37.7 | 37.8 | 37.9 | 37.7 | 38.0 | 0% |
| average O [%] | 17.6 | 17.3 | 17.2 | 17.8 | 17.8 | 2% |
| average N [%] | 0.14 | 0.16 | 0.16 | 0.14 | 0.18 | 11% |
| average S [%] | 0.05 | 0.05 | 0.05 | 0.05 | 0.06 | 9% |
| computed average H/C ratio | 1.18 | 1.18 | 1.18 | 1.17 | 1.16 | 1% |
| computed average O/C ratio | 0.47 | 0.46 | 0.45 | 0.47 | 0.47 | 2% |
| computed average N/C ratio | 0.004 | 0.004 | 0.004 | 0.004 | 0.005 | 11% |
| computed average S/C ratio | 0.001 | 0.001 | 0.001 | 0.001 | 0.002 | 37% |
| average carbon oxidation state ($C_{OS}$) | -0.233 | -0.258 | -0.259 | -0.222 | -0.212 | 9% |
| average DBE | 9.1 | 8.9 | 8.9 | 9.1 | 9.3 | 2% |
| average DBE/C | 0.46 | 0.46 | 0.47 | 0.47 | 0.47 | 1% |
| average $AI_{mod}$ | 0.30 | 0.30 | 0.30 | 0.30 | 0.31 | 1% |
| mass weighted average [Da] | 408.3 | 396.3 | 395.2 | 407.0 | 406.3 | 2% |

**Table S5.** Standard deviations of component C1 and C2-C5 for LIN, NOR, STO and MAL, acquired from EEM fluorescence measurements based on two replicates. The highest standard deviations for each sampling point (combining the five months of sampling) are reported.

| DWTP | Treatment stage | Max std C1 | Max std C2-C5 |
|---|---|---|---|
| LIN | Raw water | 0.002027 | 0.000619 |
| | Rapid sand filtr. | 0.003386 | 0.001001 |
| | Slow sand filtr. | 0.003630 | 0.005949 |
| | UV | 0.005404 | 0.001505 |
| | Chlorination | 0.006792 | 0.001948 |
| | Finished water | 0.003018 | 0.000867 |
| | Tap water | 0.008600 | 0.002771 |
| NOR | Raw water | 0.014572 | 0.043782 |
| | Coagulation | 0.001929 | 0.019418 |
| | GAC | 0.003464 | 0.015902 |
| | Slow sand filtr. | 0.006276 | 0.015408 |
| | Finished water | 0.000910 | 0.016249 |
| | Tap water | 0.002853 | 0.016026 |
| STO | Raw water | 0.013644 | 0.006051 |
| | Coagulation | 0.007772 | 0.002775 |
| | GAC | 0.013221 | 0.019643 |
| | UV | 0.004475 | 0.001372 |
| | Chloramination | 0.020626 | 0.005732 |
| | Finished water | 0.010721 | 0.003861 |
| | Tap water | 0.004174 | 0.001576 |
| MAL | Raw water | 0.004779 | 0.001105 |
| | Aeration | 0.032102 | 0.009941 |
| | Softening | 0.010560 | 0.002524 |
| | Rapid sand filtr. | 0.004191 | 0.001194 |
| | Chloramination | 0.023233 | 0.006211 |
| | Finished water | 0.012459 | 0.007084 |
| | Tap water | 0.009970 | 0.002664 |

**Table S6.** Counts of *m/z* ions and computed indices of molecular formulae detected at the different stages of water treatment in LIN throughout five sample occasions as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added). The sample points (1-7) are: 1 - Raw water, 2 - Rapid sand filtr., 3 - Slow sand filtr., 4 - UV, 5 - Chlorination, 6 - Finished water, 7 - Tap water. DBE = Double bond equivalences, $AI_{mod}$ = a modified aromaticity index.

| Characterization of DOM Mar | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
|---|---|---|---|---|---|---|---|
| number of DOM compositions | 2173 | 2203 | 2202 | 2162 | 2267 | 2216 | 2255 |
| average H [%] | 44.9 | 45.3 | 44.5 | 44.5 | 44.1 | 44.4 | 44.3 |
| average C [%] | 37.1 | 37.4 | 37.1 | 37.1 | 37.1 | 37.2 | 37.1 |
| average O [%] | 17.8 | 17.1 | 18.3 | 18.2 | 18.6 | 18.2 | 18.4 |
| average N [%] | 0.15 | 0.16 | 0.14 | 0.15 | 0.15 | 0.16 | 0.15 |
| average S [%] | 0.04 | 0.04 | 0.05 | 0.04 | 0.06 | 0.05 | 0.05 |
| computed average H/C ratio | 1.21 | 1.21 | 1.20 | 1.20 | 1.19 | 1.19 | 1.20 |
| computed average O/C ratio | 0.48 | 0.46 | 0.49 | 0.49 | 0.50 | 0.49 | 0.50 |
| computed average N/C ratio | 0.0041 | 0.0042 | 0.0039 | 0.0040 | 0.0041 | 0.0042 | 0.0040 |
| computed average S/C ratio | 0.0010 | 0.0010 | 0.0013 | 0.0012 | 0.0017 | 0.0012 | 0.0015 |
| average carbon oxidation state ($C_{OS}$) | -0.238 | -0.279 | -0.202 | -0.207 | -0.173 | -0.198 | -0.190 |
| average DBE | 8.2 | 8.2 | 8.4 | 8.4 | 8.3 | 8.3 | 8.3 |
| average DBE/C | 0.45 | 0.45 | 0.46 | 0.46 | 0.46 | 0.46 | 0.46 |
| average $AI_{mod}$ | 0.27 | 0.28 | 0.27 | 0.27 | 0.28 | 0.28 | 0.27 |
| mass weighted average [Da] | 382.3 | 373.3 | 388.0 | 387.9 | 385.3 | 380.6 | 384.3 |
| Characterization of DOM May | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
| number of DOM compositions | 2243 | 2137 | 1967 | 1917 | 1935 | 1847 | 2024 |
| average H [%] | 44.6 | 44.9 | 45.0 | 44.5 | 44.4 | 44.5 | 44.7 |
| average C [%] | 36.9 | 37.0 | 37.1 | 36.9 | 36.9 | 36.8 | 37.0 |
| average O [%] | 18.3 | 17.9 | 17.7 | 18.4 | 18.5 | 18.5 | 18.1 |
| average N [%] | 0.14 | 0.15 | 0.14 | 0.14 | 0.14 | 0.14 | 0.15 |
| average S [%] | 0.05 | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 |
| computed average H/C ratio | 1.21 | 1.21 | 1.21 | 1.21 | 1.20 | 1.21 | 1.21 |
| computed average O/C ratio | 0.50 | 0.48 | 0.48 | 0.50 | 0.50 | 0.50 | 0.49 |
| computed average N/C ratio | 0.0039 | 0.0040 | 0.0039 | 0.0037 | 0.0039 | 0.0037 | 0.0039 |
| computed average S/C ratio | 0.0013 | 0.0012 | 0.0011 | 0.0012 | 0.0012 | 0.0012 | 0.0011 |
| average carbon oxidation state ($C_{OS}$) | -0.204 | -0.230 | -0.244 | -0.200 | -0.190 | -0.192 | -0.219 |
| average DBE | 8.3 | 8.2 | 8.3 | 8.4 | 8.3 | 8.3 | 8.2 |
| average DBE/C | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 |
| average $AI_{mod}$ | 0.27 | 0.27 | 0.27 | 0.27 | 0.27 | 0.26 | 0.27 |
| mass weighted average [Da] | 389.6 | 383.4 | 385.0 | 395.7 | 390.6 | 393.3 | 384.1 |
| Characterization of DOM Aug | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
| number of DOM compositions | 2076 | 1700 | 1876 | 1898 | 1727 | 1783 | 1813 |
| average H [%] | 45.2 | 45.9 | 44.6 | 44.5 | 44.4 | 44.5 | 45.0 |
| average C [%] | 36.7 | 36.8 | 36.8 | 36.8 | 36.6 | 36.8 | 36.9 |
| average O [%] | 17.9 | 17.2 | 18.4 | 18.5 | 18.8 | 18.6 | 18.0 |
| average N [%] | 0.15 | 0.14 | 0.14 | 0.14 | 0.15 | 0.15 | 0.15 |
| average S [%] | 0.04 | 0.03 | 0.05 | 0.05 | 0.04 | 0.04 | 0.04 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| computed average H/C ratio | 1.23 | 1.25 | 1.21 | 1.21 | 1.21 | 1.21 | 1.22 |
| computed average O/C ratio | 0.49 | 0.47 | 0.50 | 0.50 | 0.51 | 0.50 | 0.49 |
| computed average N/C ratio | 0.0040 | 0.0038 | 0.0039 | 0.0038 | 0.0040 | 0.0040 | 0.0040 |
| computed average S/C ratio | 0.0012 | 0.0009 | 0.0013 | 0.0014 | 0.0011 | 0.0011 | 0.0010 |
| average carbon oxidation state ($C_{OS}$) | -0.241 | -0.298 | -0.202 | -0.192 | -0.174 | -0.189 | -0.230 |
| average DBE | 8.0 | 8.0 | 8.4 | 8.4 | 8.3 | 8.3 | 8.2 |
| average DBE/C | 0.44 | 0.43 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 |
| average $AI_{mod}$ | 0.26 | 0.26 | 0.26 | 0.26 | 0.26 | 0.26 | 0.26 |
| mass weighted average [Da] | 386.2 | 382.5 | 395.8 | 396.6 | 398.0 | 393.9 | 388.3 |
| Characterization of DOM Nov | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
| number of DOM compositions | 2080 | 2033 | 2030 | 1818 | 1731 | 1900 | 1893 |
| average H [%] | 44.8 | 44.7 | 44.5 | 44.6 | 44.6 | 44.4 | 44.2 |
| average C [%] | 36.7 | 36.7 | 36.7 | 36.6 | 36.6 | 36.7 | 36.5 |
| average O [%] | 18.3 | 18.4 | 18.6 | 18.6 | 18.5 | 18.8 | 19.1 |
| average N [%] | 0.15 | 0.15 | 0.14 | 0.13 | 0.14 | 0.14 | 0.13 |
| average S [%] | 0.05 | 0.05 | 0.06 | 0.05 | 0.04 | 0.05 | 0.06 |
| computed average H/C ratio | 1.22 | 1.22 | 1.21 | 1.22 | 1.22 | 1.21 | 1.21 |
| computed average O/C ratio | 0.50 | 0.50 | 0.51 | 0.51 | 0.51 | 0.51 | 0.52 |
| computed average N/C ratio | 0.0040 | 0.0040 | 0.0039 | 0.0036 | 0.0039 | 0.0039 | 0.0037 |
| computed average S/C ratio | 0.0014 | 0.0014 | 0.0017 | 0.0015 | 0.0012 | 0.0014 | 0.0018 |
| average carbon oxidation state ($C_{OS}$) | -0.211 | -0.202 | -0.188 | -0.191 | -0.192 | -0.172 | -0.152 |
| average DBE | 8.1 | 8.1 | 8.2 | 8.2 | 8.1 | 8.1 | 8.2 |
| average DBE/C | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 |
| average $AI_{mod}$ | 0.26 | 0.26 | 0.26 | 0.26 | 0.26 | 0.26 | 0.25 |
| mass weighted average [Da] | 383.9 | 385.6 | 388.4 | 392.3 | 388.1 | 386.4 | 393.9 |
| Characterization of DOM Jan | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
| number of DOM compositions | 1826 | 1954 | 2179 | 2221 | 2146 | 2127 | 2112 |
| average H [%] | 46.0 | 45.4 | 44.6 | 44.3 | 44.3 | 44.4 | 44.7 |
| average C [%] | 36.5 | 36.6 | 36.7 | 36.7 | 36.6 | 36.7 | 36.8 |
| average O [%] | 17.3 | 17.8 | 18.5 | 18.8 | 18.9 | 18.7 | 18.3 |
| average N [%] | 0.13 | 0.14 | 0.15 | 0.15 | 0.15 | 0.15 | 0.16 |
| average S [%] | 0.04 | 0.04 | 0.06 | 0.06 | 0.06 | 0.05 | 0.04 |
| computed average H/C ratio | 1.26 | 1.24 | 1.22 | 1.21 | 1.21 | 1.21 | 1.22 |
| computed average O/C ratio | 0.47 | 0.49 | 0.51 | 0.51 | 0.52 | 0.51 | 0.50 |
| computed average N/C ratio | 0.0036 | 0.0039 | 0.0040 | 0.0040 | 0.0040 | 0.0042 | 0.0043 |
| computed average S/C ratio | 0.0010 | 0.0011 | 0.0016 | 0.0016 | 0.0017 | 0.0013 | 0.0012 |
| average carbon oxidation state ($C_{OS}$) | -0.295 | -0.256 | -0.193 | -0.173 | -0.164 | -0.178 | -0.202 |
| average DBE | 7.9 | 8.0 | 8.2 | 8.3 | 8.2 | 8.2 | 8.1 |
| average DBE/C | 0.43 | 0.44 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 |
| average $AI_{mod}$ | 0.24 | 0.25 | 0.26 | 0.26 | 0.26 | 0.26 | 0.26 |
| mass weighted average [Da] | 390.4 | 388.6 | 393.5 | 393.0 | 391.8 | 389.9 | 384.5 |

**Table S7.** Counts of *m/z* ions and computed indices of molecular formulae detected at the different stages of water treatment in NOR throughout five sample occasions as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added). The sample points (1-6) are: 1 - Raw water. 2 - Coagulation.. 3 - GAC. 4 - Slow sand filtr.. 5 - Finished water. 6 - Tap water. DBE = Double bond equivalences. $AI_{mod}$ = a modified aromaticity index.

| Characterization of DOM Mar | P1 | P2 | P3 | P4 | P5 | P6 |
|---|---|---|---|---|---|---|
| number of DOM compositions | 2846 | 2817 | 2347 | 2447 | 2497 | 2515 |
| average H [%] | 42.9 | 45.5 | 46.3 | 45.9 | 45.8 | 45.4 |
| average C [%] | 37.8 | 37.3 | 37.3 | 37.2 | 37.2 | 37.0 |
| average O [%] | 19.0 | 16.9 | 16.2 | 16.7 | 16.8 | 17.4 |
| average N [%] | 0.14 | 0.15 | 0.13 | 0.14 | 0.14 | 0.14 |
| average S [%] | 0.09 | 0.10 | 0.07 | 0.08 | 0.07 | 0.09 |
| computed average H/C ratio | 1.14 | 1.22 | 1.24 | 1.23 | 1.23 | 1.22 |
| computed average O/C ratio | 0.50 | 0.45 | 0.43 | 0.45 | 0.45 | 0.47 |
| computed average N/C ratio | 0.0038 | 0.0039 | 0.0036 | 0.0037 | 0.0039 | 0.0038 |
| computed average S/C ratio | 0.0023 | 0.0026 | 0.0019 | 0.0021 | 0.0020 | 0.0024 |
| average carbon oxidation state ($C_{OS}$) | -0.117 | -0.298 | -0.355 | -0.318 | -0.311 | -0.272 |
| average DBE | 9.1 | 8.3 | 8.2 | 8.3 | 8.3 | 8.3 |
| average DBE/C | 0.49 | 0.45 | 0.43 | 0.44 | 0.44 | 0.44 |
| average $AI_{mod}$ | 0.31 | 0.28 | 0.27 | 0.27 | 0.27 | 0.27 |
| mass weighted average [Da] | 399.8 | 383.8 | 384.1 | 389.0 | 387.8 | 390.9 |
| Characterization of DOM May | P1 | P2 | P3 | P4 | P5 | P6 |
| number of DOM compositions | 2388 | 2601 | 2776 | 2523 | 2528 | 2235 |
| average H [%] | 43.8 | 45.7 | 45.2 | 44.9 | 45.3 | 46.2 |
| average C [%] | 38.1 | 37.4 | 37.3 | 37.2 | 37.2 | 37.4 |
| average O [%] | 18.0 | 16.7 | 17.2 | 17.8 | 17.2 | 16.3 |
| average N [%] | 0.14 | 0.14 | 0.14 | 0.14 | 0.15 | 0.14 |
| average S [%] | 0.05 | 0.08 | 0.10 | 0.09 | 0.08 | 0.05 |
| computed average H/C ratio | 1.15 | 1.22 | 1.21 | 1.21 | 1.22 | 1.24 |
| computed average O/C ratio | 0.47 | 0.45 | 0.46 | 0.48 | 0.46 | 0.44 |
| computed average N/C ratio | 0.0036 | 0.0037 | 0.0038 | 0.0037 | 0.0039 | 0.0038 |
| computed average S/C ratio | 0.0013 | 0.0021 | 0.0026 | 0.0023 | 0.0021 | 0.0014 |
| average carbon oxidation state ($C_{OS}$) | -0.189 | -0.311 | -0.275 | -0.237 | -0.274 | -0.348 |
| average DBE | 8.9 | 8.4 | 8.4 | 8.5 | 8.3 | 8.2 |
| average DBE/C | 0.48 | 0.44 | 0.45 | 0.45 | 0.45 | 0.44 |
| average $AI_{mod}$ | 0.32 | 0.28 | 0.28 | 0.27 | 0.28 | 0.28 |
| mass weighted average [Da] | 385.9 | 386.9 | 385.5 | 396.9 | 385.0 | 380.4 |
| Characterization of DOM Aug | P1 | P2 | P3 | P4 | P5 | P6 |
| number of DOM compositions | 2187 | 2231 | 2297 | 2354 | 2056 | 2234 |
| average H [%] | 44.4 | 46.8 | 46.5 | 45.3 | 45.4 | 45.7 |
| average C [%] | 37.7 | 37.2 | 37.2 | 37.0 | 36.9 | 37.0 |
| average O [%] | 17.7 | 15.8 | 16.1 | 17.5 | 17.5 | 17.2 |
| average N [%] | 0.13 | 0.14 | 0.14 | 0.14 | 0.13 | 0.14 |
| average S [%] | 0.05 | 0.06 | 0.06 | 0.08 | 0.07 | 0.06 |

| | | | | | | |
|---|---|---|---|---|---|---|
| computed average H/C ratio | 1.18 | 1.26 | 1.25 | 1.22 | 1.23 | 1.24 |
| computed average O/C ratio | 0.47 | 0.42 | 0.43 | 0.47 | 0.48 | 0.46 |
| computed average N/C ratio | 0.0035 | 0.0037 | 0.0038 | 0.0037 | 0.0036 | 0.0038 |
| computed average S/C ratio | 0.0013 | 0.0016 | 0.0016 | 0.0022 | 0.0019 | 0.0017 |
| average carbon oxidation state ($C_{OS}$) | -0.222 | -0.393 | -0.364 | -0.265 | -0.265 | -0.293 |
| average DBE | 8.7 | 8.0 | 8.1 | 8.4 | 8.2 | 8.2 |
| average DBE/C | 0.47 | 0.43 | 0.43 | 0.44 | 0.44 | 0.44 |
| average $AI_{mod}$ | 0.30 | 0.27 | 0.27 | 0.27 | 0.26 | 0.26 |
| mass weighted average [Da] | 388.3 | 378.9 | 380.8 | 395.6 | 389.7 | 388.7 |
| Characterization of DOM Nov | P1 | P2 | P3 | P4 | P5 | P6 |
| number of DOM compositions | 2362 | 2414 | 2553 | 2557 | 2334 | 2252 |
| average H [%] | 43.5 | 45.2 | 45.2 | 45.4 | 45.4 | 45.4 |
| average C [%] | 37.4 | 36.9 | 37.0 | 37.0 | 36.9 | 36.8 |
| average O [%] | 18.9 | 17.6 | 17.6 | 17.3 | 17.4 | 17.5 |
| average N [%] | 0.14 | 0.14 | 0.14 | 0.15 | 0.15 | 0.14 |
| average S [%] | 0.07 | 0.11 | 0.11 | 0.10 | 0.09 | 0.09 |
| computed average H/C ratio | 1.16 | 1.22 | 1.22 | 1.23 | 1.23 | 1.23 |
| computed average O/C ratio | 0.50 | 0.48 | 0.47 | 0.47 | 0.47 | 0.48 |
| computed average N/C ratio | 0.0037 | 0.0037 | 0.0039 | 0.0040 | 0.0040 | 0.0039 |
| computed average S/C ratio | 0.0020 | 0.0031 | 0.0030 | 0.0028 | 0.0024 | 0.0023 |
| average carbon oxidation state ($C_{OS}$) | -0.139 | -0.256 | -0.258 | -0.275 | -0.271 | -0.265 |
| average DBE | 8.8 | 8.3 | 8.3 | 8.2 | 8.2 | 8.2 |
| average DBE/C | 0.47 | 0.44 | 0.44 | 0.44 | 0.44 | 0.44 |
| average $AI_{mod}$ | 0.29 | 0.27 | 0.27 | 0.27 | 0.26 | 0.26 |
| mass weighted average [Da] | 396.4 | 393.4 | 391.2 | 388.1 | 387.4 | 391.4 |
| Characterization of DOM Jan | P1 | P2 | P3 | P4 | P5 | P6 |
| number of DOM compositions | 2859 | 2901 | 2665 | 2771 | 2546 | 2577 |
| average H [%] | 42.7 | 45.1 | 46.0 | 45.4 | 45.5 | 45.3 |
| average C [%] | 37.4 | 37.0 | 37.0 | 36.9 | 36.9 | 36.9 |
| average O [%] | 19.6 | 17.7 | 16.8 | 17.4 | 17.3 | 17.6 |
| average N [%] | 0.14 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 |
| average S [%] | 0.11 | 0.14 | 0.11 | 0.12 | 0.10 | 0.10 |
| computed average H/C ratio | 1.14 | 1.22 | 1.24 | 1.23 | 1.23 | 1.23 |
| computed average O/C ratio | 0.52 | 0.48 | 0.45 | 0.47 | 0.47 | 0.48 |
| computed average N/C ratio | 0.0038 | 0.0039 | 0.0039 | 0.0041 | 0.0041 | 0.0040 |
| computed average S/C ratio | 0.0030 | 0.0037 | 0.0029 | 0.0031 | 0.0028 | 0.0028 |
| average carbon oxidation state ($C_{OS}$) | -0.0825 | -0.2470 | -0.3171 | -0.2731 | -0.2758 | -0.2544 |
| average DBE | 9.1 | 8.4 | 8.1 | 8.2 | 8.2 | 8.2 |
| average DBE/C | 0.48 | 0.45 | 0.43 | 0.44 | 0.44 | 0.44 |
| average $AI_{mod}$ | 0.29 | 0.27 | 0.26 | 0.26 | 0.26 | 0.26 |
| mass weighted average [Da] | 407.2 | 395.1 | 384.5 | 387.0 | 387.9 | 392.8 |

**Table S8.** Counts of *m/z* ions and computed indices of molecular formulae detected at the different stages of water treatment in STO throughout five sample occasions as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added). The sample points (1-7) are: 1 - Raw water. 2 - Coagulation. 3 - GAC. 4 - UV. 5 - Chloramination. 6 - Finished water. 7 - Tap water. DBE = Double bond equivalences. $AI_{mod}$ = a modified aromaticity index.

| Characterization of DOM Mar | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
|---|---|---|---|---|---|---|---|
| number of DOM compositions | 2185 | 2032 | 2309 | 2835 | 2289 | 2406 | 2630 |
| average H [%] | 42.9 | 44.7 | 44.6 | 45.5 | 44.7 | 44.9 | 45.3 |
| average C [%] | 37.4 | 37.0 | 37.0 | 37.2 | 36.9 | 36.9 | 37.1 |
| average O [%] | 19.5 | 18.1 | 18.2 | 17.1 | 18.1 | 18.0 | 17.4 |
| average N [%] | 0.11 | 0.09 | 0.10 | 0.13 | 0.10 | 0.14 | 0.14 |
| average S [%] | 0.08 | 0.11 | 0.13 | 0.08 | 0.12 | 0.09 | 0.08 |
| computed average H/C ratio | 1.15 | 1.21 | 1.21 | 1.23 | 1.21 | 1.22 | 1.22 |
| computed average O/C ratio | 0.52 | 0.49 | 0.49 | 0.46 | 0.49 | 0.49 | 0.47 |
| computed average N/C ratio | 0.0029 | 0.0024 | 0.0026 | 0.0036 | 0.0028 | 0.0037 | 0.0037 |
| computed average S/C ratio | 0.0022 | 0.0031 | 0.0035 | 0.0022 | 0.0032 | 0.0026 | 0.0022 |
| average carbon oxidation state ($C_{OS}$) | -0.095 | -0.213 | -0.210 | -0.291 | -0.215 | -0.228 | -0.266 |
| average DBE | 9.3 | 8.6 | 8.7 | 8.5 | 8.7 | 8.7 | 8.6 |
| average DBE/C | 0.48 | 0.45 | 0.45 | 0.44 | 0.45 | 0.45 | 0.44 |
| average $AI_{mod}$ | 0.29 | 0.27 | 0.27 | 0.27 | 0.26 | 0.26 | 0.27 |
| mass weighted average [Da] | 417.3 | 407.8 | 410.8 | 398.7 | 411.2 | 411.3 | 403.2 |
| Characterization of DOM May | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
| number of DOM compositions | 2719 | 2762 | 2640 | 1534 | 2774 | 1648 | 1678 |
| average H [%] | 44.7 | 45.5 | 46.0 | 46.1 | 46.2 | 46.3 | 46.4 |
| average C [%] | 37.7 | 37.2 | 37.1 | 36.9 | 37.2 | 37.0 | 37.0 |
| average O [%] | 17.4 | 17.1 | 16.8 | 16.9 | 16.4 | 16.6 | 16.4 |
| average N [%] | 0.15 | 0.13 | 0.14 | 0.12 | 0.15 | 0.11 | 0.11 |
| average S [%] | 0.05 | 0.08 | 0.06 | 0.04 | 0.06 | 0.04 | 0.04 |
| computed average H/C ratio | 1.18 | 1.22 | 1.24 | 1.25 | 1.24 | 1.25 | 1.26 |
| computed average O/C ratio | 0.46 | 0.46 | 0.45 | 0.46 | 0.44 | 0.45 | 0.44 |
| computed average N/C ratio | 0.0039 | 0.0035 | 0.0039 | 0.0033 | 0.0039 | 0.0029 | 0.0030 |
| computed average S/C ratio | 0.0013 | 0.0022 | 0.0017 | 0.0011 | 0.0016 | 0.0012 | 0.0012 |
| average carbon oxidation state ($C_{OS}$) | -0.245 | -0.288 | -0.320 | -0.321 | -0.341 | -0.339 | -0.351 |
| average DBE | 8.8 | 8.5 | 8.4 | 8.3 | 8.3 | 8.3 | 8.2 |
| average DBE/C | 0.46 | 0.44 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 |
| average $AI_{mod}$ | 0.30 | 0.27 | 0.26 | 0.26 | 0.27 | 0.26 | 0.26 |
| mass weighted average [Da] | 392.5 | 398.0 | 400.1 | 400.3 | 391.5 | 396.1 | 395.7 |
| Characterization of DOM Aug | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
| number of DOM compositions | 1688 | 1687 | 1412 | 1187 | 1119 | 1269 | 1523 |
| average H [%] | 43.5 | 46.1 | 45.9 | 45.3 | 45.2 | 45.3 | 45.2 |
| average C [%] | 37.3 | 37.0 | 37.0 | 36.9 | 36.8 | 36.9 | 36.9 |
| average O [%] | 19.0 | 16.8 | 17.0 | 17.6 | 17.8 | 17.7 | 17.8 |
| average N [%] | 0.10 | 0.10 | 0.09 | 0.07 | 0.07 | 0.08 | 0.09 |
| average S [%] | 0.05 | 0.05 | 0.04 | 0.05 | 0.05 | 0.06 | 0.06 |

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|---|---|---|---|---|---|---|---|
| computed average H/C ratio | 1.16 | 1.24 | 1.24 | 1.23 | 1.23 | 1.23 | 1.22 |
| computed average O/C ratio | 0.51 | 0.45 | 0.46 | 0.48 | 0.48 | 0.48 | 0.48 |
| computed average N/C ratio | 0.0026 | 0.0027 | 0.0025 | 0.0020 | 0.0019 | 0.0021 | 0.0023 |
| computed average S/C ratio | 0.0013 | 0.0013 | 0.0011 | 0.0013 | 0.0013 | 0.0015 | 0.0017 |
| average carbon oxidation state ($C_{OS}$) | -0.133 | -0.323 | -0.305 | -0.262 | -0.249 | -0.255 | -0.248 |
| average DBE | 9.0 | 8.3 | 8.2 | 8.2 | 8.2 | 8.2 | 8.4 |
| average DBE/C | 0.47 | 0.43 | 0.43 | 0.44 | 0.44 | 0.44 | 0.44 |
| average $AI_{mod}$ | 0.29 | 0.26 | 0.26 | 0.26 | 0.26 | 0.26 | 0.26 |
| mass weighted average [Da] | 407.8 | 397.1 | 393.0 | 390.8 | 390.0 | 392.4 | 399.1 |
| Characterization of DOM Nov | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
| number of DOM compositions | 1589 | 1696 | 1581 | 2139 | 1406 | 2902 | 2717 |
| average H [%] | 43.1 | 44.7 | 45.1 | 45.3 | 45.6 | 45.2 | 45.8 |
| average C [%] | 37.3 | 37.0 | 37.0 | 37.1 | 36.9 | 37.0 | 37.1 |
| average O [%] | 19.4 | 18.1 | 17.8 | 17.5 | 17.4 | 17.6 | 16.9 |
| average N [%] | 0.09 | 0.09 | 0.09 | 0.11 | 0.08 | 0.13 | 0.14 |
| average S [%] | 0.05 | 0.07 | 0.06 | 0.07 | 0.05 | 0.10 | 0.07 |
| computed average H/C ratio | 1.16 | 1.21 | 1.22 | 1.22 | 1.24 | 1.22 | 1.24 |
| computed average O/C ratio | 0.52 | 0.49 | 0.48 | 0.47 | 0.47 | 0.48 | 0.45 |
| computed average N/C ratio | 0.0025 | 0.0025 | 0.0024 | 0.0030 | 0.0022 | 0.0036 | 0.0037 |
| computed average S/C ratio | 0.0014 | 0.0019 | 0.0017 | 0.0018 | 0.0014 | 0.0026 | 0.0019 |
| average carbon oxidation state ($C_{OS}$) | -0.106 | -0.218 | -0.243 | -0.261 | -0.275 | -0.258 | -0.310 |
| average DBE | 8.9 | 8.5 | 8.4 | 8.6 | 8.2 | 8.4 | 8.3 |
| average DBE/C | 0.48 | 0.45 | 0.44 | 0.44 | 0.44 | 0.44 | 0.44 |
| average $AI_{mod}$ | 0.29 | 0.27 | 0.27 | 0.27 | 0.26 | 0.27 | 0.27 |
| mass weighted average [Da] | 404.2 | 400.2 | 398.0 | 404.7 | 394.1 | 395.2 | 392.2 |
| Characterization of DOM Jan | P1 | P2 | P3 | P4 | P5 | P6 | P7 |
| number of DOM compositions | 2198 | 2214 | 2237 | 2194 | 2206 | 2048 | 2021 |
| average H [%] | 43.0 | 44.7 | 44.8 | 44.8 | 44.7 | 44.8 | 44.8 |
| average C [%] | 37.3 | 36.9 | 36.9 | 36.9 | 36.8 | 36.8 | 36.8 |
| average O [%] | 19.5 | 18.2 | 18.1 | 18.1 | 18.3 | 18.2 | 18.2 |
| average N [%] | 0.10 | 0.10 | 0.10 | 0.09 | 0.10 | 0.09 | 0.09 |
| average S [%] | 0.09 | 0.12 | 0.11 | 0.11 | 0.12 | 0.12 | 0.11 |
| computed average H/C ratio | 1.15 | 1.21 | 1.21 | 1.21 | 1.21 | 1.22 | 1.22 |
| computed average O/C ratio | 0.52 | 0.49 | 0.49 | 0.49 | 0.50 | 0.49 | 0.49 |
| computed average N/C ratio | 0.0026 | 0.0026 | 0.0026 | 0.0025 | 0.0026 | 0.0024 | 0.0025 |
| computed average S/C ratio | 0.0025 | 0.0033 | 0.0030 | 0.0030 | 0.0033 | 0.0032 | 0.0030 |
| average carbon oxidation state ($C_{OS}$) | -0.098 | -0.210 | -0.220 | -0.217 | -0.205 | -0.213 | -0.214 |
| average DBE | 9.1 | 8.5 | 8.6 | 8.6 | 8.6 | 8.5 | 8.5 |
| average DBE/C | 0.48 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 |
| average $AI_{mod}$ | 0.29 | 0.26 | 0.27 | 0.27 | 0.26 | 0.26 | 0.26 |
| mass weighted average [Da] | 414.1 | 406.1 | 407.8 | 407.8 | 408.9 | 406.7 | 406.0 |

**Table S9.** Counts of *m/z* ions and computed indices of molecular formulae detected at the different stages of water treatment in MAL throughout five sample occasions as computed from negative electrospray 12T FT-ICR mass spectra for singly charged ions reported in neutral form (the mass of a proton added). The sample points (1-8) are: 1 - Raw water. 2 - Aeration. 3 - Softening. 4 - Rapid sand filtr.. 5 - UV. 6 - Chloramination 7 - Finished water. 8 - Tap water. DBE = Double bond equivalences. $AI_{mod}$ = a modified aromaticity index.

| Characterization of DOM Mar | P1 | P2 | P3 | P4 | P5 | P6 | P7 | P8 |
|---|---|---|---|---|---|---|---|---|
| number of DOM compositions | 2062 | 2157 | 2276 | 2278 | NA | 2164 | 2036 | 2029 |
| average H [%] | 44.4 | 44.3 | 43.9 | 44.1 | NA | 44.4 | 44.7 | 44.3 |
| average C [%] | 37.7 | 37.8 | 37.9 | 38.0 | NA | 37.9 | 37.9 | 37.3 |
| average O [%] | 17.6 | 17.7 | 17.9 | 17.6 | NA | 17.5 | 17.3 | 18.0 |
| average N [%] | 0.14 | 0.16 | 0.19 | 0.18 | NA | 0.17 | 0.17 | 0.22 |
| average S [%] | 0.05 | 0.05 | 0.06 | 0.06 | NA | 0.05 | 0.04 | 0.11 |
| computed average H/C ratio | 1.18 | 1.17 | 1.16 | 1.16 | NA | 1.17 | 1.18 | 1.19 |
| computed average O/C ratio | 0.47 | 0.47 | 0.47 | 0.46 | NA | 0.46 | 0.46 | 0.48 |
| computed average N/C ratio | 0.0038 | 0.0043 | 0.0049 | 0.0048 | NA | 0.0046 | 0.0045 | 0.0058 |
| computed average S/C ratio | 0.0014 | 0.0014 | 0.0015 | 0.0015 | NA | 0.0013 | 0.0011 | 0.0029 |
| average carbon oxidation state ($C_{OS}$) | -0.233 | -0.228 | -0.205 | -0.224 | NA | -0.237 | -0.256 | -0.212 |
| average DBE | 9.1 | 9.1 | 9.2 | 9.1 | NA | 9.0 | 8.9 | 8.7 |
| average DBE/C | 0.46 | 0.47 | 0.48 | 0.47 | NA | 0.47 | 0.46 | 0.46 |
| average $AI_{mod}$ | 0.30 | 0.30 | 0.31 | 0.31 | NA | 0.30 | 0.30 | 0.29 |
| mass weighted average [Da] | 408.3 | 404.8 | 402.2 | 400.2 | NA | 398.3 | 396.3 | 398.1 |
| Characterization of DOM May | P1 | P2 | P3 | P4 | P5 | P6 | P7 | P8 |
| number of DOM compositions | 2106 | 2209 | 2254 | 2117 | NA | 1999 | 1914 | 1921 |
| average H [%] | 44.7 | 44.2 | 43.8 | 44.0 | NA | 44.2 | 44.5 | 44.5 |
| average C [%] | 37.8 | 38.1 | 37.8 | 37.8 | NA | 37.7 | 37.6 | 37.4 |
| average O [%] | 17.3 | 17.5 | 18.1 | 18.0 | NA | 17.9 | 17.7 | 17.9 |
| average N [%] | 0.16 | 0.17 | 0.18 | 0.18 | NA | 0.17 | 0.17 | 0.20 |
| average S [%] | 0.05 | 0.06 | 0.07 | 0.06 | NA | 0.05 | 0.05 | 0.08 |
| computed average H/C ratio | 1.18 | 1.16 | 1.16 | 1.16 | NA | 1.17 | 1.18 | 1.19 |
| computed average O/C ratio | 0.46 | 0.46 | 0.48 | 0.47 | NA | 0.47 | 0.47 | 0.48 |
| computed average N/C ratio | 0.0041 | 0.0044 | 0.0046 | 0.0047 | NA | 0.0046 | 0.0046 | 0.0054 |
| computed average S/C ratio | 0.0013 | 0.0015 | 0.0018 | 0.0015 | NA | 0.0014 | 0.0014 | 0.0022 |
| average carbon oxidation state ($C_{OS}$) | -0.258 | -0.234 | -0.193 | -0.204 | NA | -0.213 | -0.229 | -0.225 |
| average DBE | 8.9 | 9.1 | 9.1 | 9.2 | NA | 9.0 | 8.9 | 8.7 |
| average DBE/C | 0.46 | 0.47 | 0.47 | 0.47 | NA | 0.47 | 0.46 | 0.46 |
| average $AI_{mod}$ | 0.30 | 0.31 | 0.30 | 0.30 | NA | 0.30 | 0.29 | 0.29 |
| mass weighted average [Da] | 396.3 | 396.6 | 403.3 | 404.3 | NA | 400.2 | 399.6 | 397.8 |
| Characterization of DOM Aug | P1 | P2 | P3 | P4 | P5 | P6 | P7 | P8 |
| number of DOM compositions | 2108 | 2047 | 2230 | 2135 | NA | 1930 | 1945 | 1901 |
| average H [%] | 44.7 | 44.2 | 44.0 | 43.8 | NA | 44.0 | 44.2 | 44.1 |
| average C [%] | 37.9 | 37.8 | 37.9 | 37.7 | NA | 37.5 | 37.6 | 37.4 |
| average O [%] | 17.2 | 17.8 | 17.9 | 18.3 | NA | 18.3 | 17.9 | 18.2 |
| average N [%] | 0.16 | 0.15 | 0.18 | 0.17 | NA | 0.17 | 0.16 | 0.19 |
| average S [%] | 0.05 | 0.05 | 0.06 | 0.07 | NA | 0.05 | 0.05 | 0.07 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| computed average H/C ratio | 1.18 | 1.17 | 1.16 | 1.16 | NA | 1.17 | 1.18 | 1.18 |
| computed average O/C ratio | 0.45 | 0.47 | 0.47 | 0.48 | NA | 0.49 | 0.48 | 0.49 |
| computed average N/C ratio | 0.0043 | 0.0041 | 0.0048 | 0.0045 | NA | 0.0044 | 0.0043 | 0.0050 |
| computed average S/C ratio | 0.0013 | 0.0013 | 0.0016 | 0.0019 | NA | 0.0014 | 0.0012 | 0.0018 |
| average carbon oxidation state ($C_{OS}$) | -0.259 | -0.216 | -0.207 | -0.183 | NA | -0.189 | -0.212 | -0.197 |
| average DBE | 8.9 | 9.2 | 9.1 | 9.1 | NA | 9.0 | 9.0 | 8.9 |
| average DBE/C | 0.47 | 0.47 | 0.47 | 0.47 | NA | 0.47 | 0.47 | 0.46 |
| average $AI_{mod}$ | 0.30 | 0.30 | 0.31 | 0.30 | NA | 0.29 | 0.29 | 0.29 |
| mass weighted average [Da] | 395.2 | 407.5 | 400.9 | 406.2 | NA | 405.1 | 405.5 | 405.5 |
| Characterization of DOM Nov | P1 | P2 | P3 | P4 | P5 | P6 | P7 | P8 |
| number of DOM compositions | 1927 | 1872 | 2071 | 2070 | 2181 | 1881 | 2021 | 1902 |
| average H [%] | 44.3 | 43.8 | 43.6 | 43.6 | 43.6 | 43.7 | 44.1 | 44.5 |
| average C [%] | 37.7 | 37.8 | 37.8 | 37.7 | 37.7 | 37.5 | 37.6 | 37.4 |
| average O [%] | 17.8 | 18.2 | 18.5 | 18.4 | 18.4 | 18.6 | 18.1 | 17.8 |
| average N [%] | 0.14 | 0.15 | 0.17 | 0.17 | 0.16 | 0.16 | 0.17 | 0.23 |
| average S [%] | 0.05 | 0.06 | 0.07 | 0.07 | 0.08 | 0.06 | 0.05 | 0.07 |
| computed average H/C ratio | 1.17 | 1.16 | 1.15 | 1.16 | 1.16 | 1.16 | 1.17 | 1.19 |
| computed average O/C ratio | 0.47 | 0.48 | 0.49 | 0.49 | 0.49 | 0.50 | 0.48 | 0.48 |
| computed average N/C ratio | 0.0038 | 0.0039 | 0.0044 | 0.0044 | 0.0044 | 0.0042 | 0.0045 | 0.0062 |
| computed average S/C ratio | 0.0014 | 0.0015 | 0.0018 | 0.0018 | 0.0020 | 0.0016 | 0.0014 | 0.0019 |
| average carbon oxidation state ($C_{OS}$) | -0.222 | -0.188 | -0.168 | -0.173 | -0.171 | -0.165 | -0.199 | -0.226 |
| average DBE | 9.1 | 9.3 | 9.3 | 9.2 | 9.2 | 9.1 | 9.0 | 8.7 |
| average DBE/C | 0.47 | 0.47 | 0.48 | 0.48 | 0.48 | 0.47 | 0.47 | 0.46 |
| average $AI_{mod}$ | 0.30 | 0.30 | 0.30 | 0.30 | 0.30 | 0.29 | 0.29 | 0.29 |
| mass weighted average [Da] | 407.0 | 411.8 | 410.8 | 409.9 | 409.1 | 411.3 | 404.1 | 395.4 |
| Characterization of DOM Jan | P1 | P2 | P3 | P4 | P5 | P6 | P7 | P8 |
| number of DOM compositions | 2318 | 2270 | 2123 | 2095 | 2171 | 2072 | 2136 | 1960 |
| average H [%] | 44.0 | 43.9 | 44.1 | 44.1 | 44.1 | 44.4 | 44.1 | 45.4 |
| average C [%] | 38.0 | 37.9 | 37.8 | 37.7 | 37.7 | 37.5 | 37.5 | 37.0 |
| average O [%] | 17.8 | 18.0 | 17.9 | 17.9 | 18.0 | 18.0 | 18.2 | 17.4 |
| average N [%] | 0.18 | 0.17 | 0.18 | 0.17 | 0.18 | 0.16 | 0.17 | 0.10 |
| average S [%] | 0.06 | 0.06 | 0.06 | 0.06 | 0.06 | 0.06 | 0.07 | 0.10 |
| computed average H/C ratio | 1.16 | 1.16 | 1.17 | 1.17 | 1.17 | 1.18 | 1.17 | 1.23 |
| computed average O/C ratio | 0.47 | 0.48 | 0.47 | 0.48 | 0.48 | 0.48 | 0.49 | 0.47 |
| computed average N/C ratio | 0.0047 | 0.0045 | 0.0047 | 0.0046 | 0.0047 | 0.0043 | 0.0044 | 0.0027 |
| computed average S/C ratio | 0.0015 | 0.0017 | 0.0015 | 0.0017 | 0.0017 | 0.0016 | 0.0018 | 0.0026 |
| average carbon oxidation state ($C_{OS}$) | -0.212 | -0.199 | -0.210 | -0.208 | -0.206 | -0.215 | -0.195 | -0.273 |
| average DBE | 9.3 | 9.3 | 9.2 | 9.1 | 9.1 | 8.9 | 9.0 | 8.2 |
| average DBE/C | 0.47 | 0.47 | 0.47 | 0.47 | 0.47 | 0.46 | 0.47 | 0.44 |
| average $AI_{mod}$ | 0.31 | 0.30 | 0.30 | 0.30 | 0.30 | 0.29 | 0.29 | 0.27 |
| mass weighted average [Da] | 406.3 | 408.8 | 408.1 | 406.0 | 403.9 | 402.0 | 404.2 | 389.6 |

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