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Insights into NOM quality changes by combination of easy designed experiments close to nature and monitoring using FT-ICR-MS

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Natural organic matter (NOM) is often still a black box considering its isomeric composition. From the analytical point of view the highest resolution of NOM can be achieved by Fourier-transform ion cyclotron resonance mass spectroscopy (FT-ICR-MS). This analytical tool generates elemental compositions of thousands of NOM components (molecular formulas, MFs) which can be extracted from aqueous samples (e.g., via solid phase extraction) and which are ionizable (e.g. via electrospray ionization). The comparison of NOM quality in waters of different ecosystems has generated useful insights about ecosystem-specific molecular differences. However, NOM is not an inert mixture of compounds and can undergo chemical changes by photochemical or microbial reactions or adsorptive fractionation. By following the relative intensity changes of single MFs during simple experiments close to nature or monitoring, elucidation of the reactivity of the underlying NOM compounds is possible.

We have combined a photochemical degradation experiment close to nature with monitoring results from two German drinking water reservoirs with the perspective to disentangle photochemical and microbial reactions in the reservoirs. Bacterial induced transformations were widely excluded in the photo degradation experiment by filtration of the sample water before irradiation. During the reservoir monitoring, both microbial and photochemical reactions can be suggested from relative intensity differences of single MFs during lake stratification (between epi- and hypolimnion). MFs show intensity changes both in the photo experiment and in the lake monitoring are regarded as photo labile or photo products. Those MFs with intensity differences only in the lake monitoring can be regarded as microbial reactive.

A great number of highly reactive MFs were found to be present in all samples of both the photo degradation experiment and the lake monitoring. MFs like $C_9H_{12}O_6$, $C_{10}H_{14}O_6$, $C_{10}H_{14}O_7$, $C_{11}H_{16}O_5$ were photo products, MFs like $C_{20}H_{16}O_{14}$, $C_{19}H_{14}O_{13}$, $C_{18}H_{12}O_{12}$ were photo degraded. MFs like $C_{10}H_{10}O_7$ and $C_9H_{10}O_7$ could be suggested to be microbial products because they showed elevated intensity in epilimnetic waters but minor reactivity in the photo experiment.

Our studies (1, 2, 3) provide the attempt to follow NOM reactivity by visualization of single MFs relative intensities versus time and / or space.

1) Wilske, C.et al.,Water MDPI (2020) 12 (2).

2) Herzsprung P. et al., Environ. Sci. Technol. (2020), 54, 13556-13565

3) Wilske C. et al., Water MDPI (2021), 13, 1703.