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Shedding light into the forest: improved understanding of DOM processing in freshwater using complementary experimental and machine learning approaches

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Dissolved organic matter (DOM) plays important roles in aquatic ecosystems but can interfere with drinking water production. However, its highly complex composition and chemical diversity makes it difficult to understand molecular reactivity in natural systems. Here we used ultra-high resolution mass spectrometry (FT-ICR-MS) and data from two independent studies (a lake monitoring and a photo-irradiation experiment) to disentangle DOM reactivity based on photochemical and microbial induced transformations.

Monitoring in Germany' largest drinking water reservoir (Rappbode reservoir, Harz Mountains) was conducted over one year on seven dates using water from nine depths. Water chemistry and limnological parameters, including chlorophyll a (chl a) concentration were determined. Stratification of the lake allowed to determine depths and periods, where an accumulation of chl a corresponded with an accumulation of DOM compounds. Chl a served as a surrogate for microbially (i.e. primary) produced DOM. In addition, we used data from a photodegradation experiment using river water from a catchment with similar land use (tributary to Muldenberg reservoir in the Ore Mountains, Germany). The water had been irradiated for 6 days in triplicates using natural sunlight. Thirteen time points had been sampled and used to determine the photochemical reactivity of DOM compounds.

We used robust rank correlations to establish relationships between predictor (chl a concentration or cumulated sunlight irradiation) and response variables (normalized FT-ICR mass peak intensities) for each dataset. Combining the resulting data further allowed for an orthogonal classification of 1277 molecular formulas, which were present in all samples. Using this approach, we could identify 11 reactivity groups and attributed chemical properties to these groups based on molecular information. Photodegradation was observed for high molecular weight molecules - similar to microbial degradation - whereas photo products were aliphatic and oxygen rich. We found that in the lake studied, DOM turnover was dominated by photochemical processes. Exclusively microbial products were comparably low in number and of small molecular weight

compounds.

Based on the molecular-property-reactivity-relationships, we trained a random forest model and predicted the molecular reactivity for the remainder of molecular formulas, for which insufficient data were initially available.

The approach presented here offers an expandable tool to integrate reactivity of DOM from specific environments and link it to its molecular properties and chemistry. This will lead to enhanced understanding of the ecological function and biogeochemical cycling of DOM.