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Identification of ecosystem-specific markers in dissolved organic matter by Orbitrap tandem mass spectrometry

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Dissolved organic matter (DOM) integrates signatures of 1) biota and biotic interactions, like plant and microbial community structure and food webs, 2) geology, as mineral composition, sorption processes and nutrient content, and 3) climate, like water balance, groundwater levels or temperature. These factors change in space and time, e.g. through seasonality, rewetting cycles and extreme events, and are modified through human impact, as land-use changes or fertilization. Ultrahigh resolution mass spectrometry (Fourier Transform Mass Spectrometry, FTMS) has opened up the “black box” of molecular-level DOM information. Through FTMS studies, it became apparent that ecosystem DOM fingerprints are complex and composed of both ubiquitous signals and specific signals possibly linked to rather “common” or “unique” types of ecosystem information. However, compound group and chemical structure annotations based on sum formulae remain preliminary and chemically imprecise as multiple structural isomers exist for a single mass and identification by current mass spectrometric databases often cannot be achieved. This directly limits our capability to link ecosystems and ecosystem processes to molecules and new approaches are needed to improve our possibilities to identify unknown structures.

Analyses of mass spectrometric fragmentation patterns using the tandem mass spectrometry (MSn) option of FTMS instruments unlock potential to identify these unknown ecosystem markers. In a recent study that analyzed DOM from bogs, rivers, and soils of coniferous, mixed, deciduous forests and grasslands ecosystems, Roth et al. (2014) identified tannin formulae by their O/C and H/C ratios as possible forest markers. Here we conducted MSn experiments with an Orbitrap Elite mass spectrometer and performed mass spectrometric fragmentation experiments on standard compounds to confirm this identification. We present fragmentation patterns from tannin-related structures, phenolic structures, like lignin monomers and other methoxy-phenols and quinones and compared them to the fragmentation patterns of the “tannin-like” forest markers.

References

Roth, V.-N., Dittmar, T., Gaupp, R. & G. Gleixner (2014): Ecosystem-specific composition of dissolved organic matter. Vadose Zone J. 13. doi:10.2136/vzj2013.09.0162