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Thermodynamic indicators decipher the molecular composition of organic matter in phase transition

Philipp Maurischat[1], Michael Seidel[2], Oliver Donnerhack[3], Patrick Liebmann[3], and Georg Guggenberger[3]
[1]Institute for Biology and Environmental Sciences (IBU), Carl von Ossietzky Universität Oldenburg, Germany
[2]Institute for Chemistry and Biology of the Marine Environment (ICBM), Carl von Ossietzky Universität Oldenburg, Germany
[3]Institute of Soil Science, Leibniz University Hannover, Germany

With promising methods such as ultrahigh-resolution mass spectrometry (FT ICR MS), soil scientists have more opportunity than ever to gain a comprehensive picture of the composition and transformation of soil organic matter (SOM). With soils as central mediators for carbon capture and storage this understanding is key when it comes to tackling major challenges, such as climate change and soil health. However, as novel techniques are often imported from other scientific fields, the evaluation and interpretation of data with regard to the heterogeneous pedosphere often remains a major challenge. For FT ICR MS, several commonly used indices were developed from empirical observations of the deep ocean. While these indices seem statistically transferable from ocean DOM to the terrestrial realm, there is legitimate concern that no causality ultimately ensures this applicability. Indices are needed that allow interpretation of the data from a conceptual perspective. Viewing SOM as a thermodynamically driven mediator of energy fluxes in the soil food web provides an opportunity to put a foot on the ground of data analysis with more general applicability. We aim to show that bioenergetic and thermodynamic molecular indices allow a better understanding of soil organic matter transformation by comparing FT ICR MS samples from complex, mixed sources and single source endmembers.

We investigated the molecular composition of stream DOM and soil leachates along a biome gradient between alpine meadow and alpine steppe, including a chronosequence of degradation in the southern Tibetan Nam Co watershed. Our results suggest a certain match of commonly used DOM molecular indices, such as the ‘island of stability‘, the ‘degradation index‘ and the ‘terrestrial index‘, applied to marine settings for terrestrial DOM and SOM. However, when comparing SOM and DOM phase transitions within endmember sources, we noted inconsistencies. In contrast, indicators representing the bioenergetics of organic matter composition, such as the ‘nominal oxidation state of carbon’ and the ‘Gibbs free energy for carbon oxidation’, show good agreement for the key phase transition between SOM and DOM. These results provide reasonable evidence in line with conceptual understanding, such as more oxidised DOM and SOM in degraded areas and generally less oxidised molecular formulae in mainly allochthonous stream DOM compared to extracted SOM. Our data support the notion that bioenergetic and thermodynamic indicators may be a way forward to better understand the

complex nature of organic matter transformation in soils with FT ICR MS. These indicators can serve as important building blocks for molecular fingerprinting.