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A Multi-Trait, Substrate-Explicit Thermodynamic Modeling Framework to Identify and Characterize Bioavailable Organic Matter Across River Corridors

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Molecular fingerprinting of environmental organic matter through Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry (FTICR-MS) grants rich datasets composed of thousands of unique molecular formulae. The WHONDRS Summer 2019 Sampling Campaign yielded a rich set of FTICR-MS profiles from surface water and river sediments, which when analyzed with substrate-explicit thermodynamic modeling, also known as lambda modeling, previously identified key chemical and thermodynamic traits governing organic matter bioavailability. Given samples were collected from diverse ecosystems, with different physical environmental (temperature, pH, etc.), and diverse microbial communities with distinct genetic potential, the model alone does not account for sample-specific differences influencing respiration of organic matter. Therefore, we expanded upon the lambda model, incorporating sample-specific physical, chemical, and biological features into the lambda modeling framework. Microbial aerobic respiration through this approach was additionally represented as a continuous function of key chemical, thermodynamic, and biological features, representing predicted bioavailability quantitatively, building upon the lambda model's previous qualitative (binary) categorization of bioavailable organic matter. With both qualitative and quantitative approaches resulted in improved model predicted respiration compared to the campaign's measured aerobic respiration rates (Binary: $r = 0.77$, $p<0.05$; Continuous: $r = 0.79$, $p<0.05$). For further contextualization of bioavailability, we assessed the compound classes, putative molecular transformations, and metagenome functional gene richness associated with samples and co-occurrent compounds. Through this approach we found lipids and phytochemicals, despite representing over 80% of the total molecular richness across samples, had comparably low average bioavailability to compound classes of lower richness such as carbohydrates and proteins. This integrative analysis and quantitative predictions of bioavailability aim to improve compatibility with existing biogeochemical and reactive transport models, for future interpretable and scalable simulations of biogeochemical processes.