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Natural Organic Matter and our Current Capacity to Depict Molecular Dissimilarity

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Terrestrial natural organic compounds divide into functional biomolecules which eventually derive from a genetic code and complex biogeochemical non-repetitive materials, like natural organic matter (NOM), which are formed according to the general constraints of thermodynamics and kinetics from molecules of geochemical or ultimately biogenic origin. The combined action of biotic and abiotic reactions characteristic of the respective ecosystems progressively attenuates original biosignatures and the resulting diversity of NOM molecular signatures approaches the limits constrained by the laws of chemical binding.

Successful non-target molecular-level analyses of NOM often require integration of high-performance separation, high-resolution organic structural spectroscopy and mathematical data treatment. High-precision frequency measurements are at the core of the two most influential methods of organic structural spectroscopy for the investigation of complex organic materials, NMR spectroscopy (provide unsurpassed insight into close-range molecular order) and FTICR mass spectrometry (provide depiction of the compositional space with unsurpassed resolution), and can be translated into isotope-specific molecular resolution detail of unprecedented significance and richness. The currently available discrete analytical volumetric pixel space to describe complex systems (which is defined by NMR, FT mass spectrometry and separation technology) is in the range of 10E8-10E14 voxels and therefore capable to provide the necessary detail for a meaningful molecular level analysis of very complex mixtures.

This presentation uses recent examples of complementary high-resolution organic structural spectroscopy to elucidate key structural aspects of various NOM. Soil-derived, freshwater, marine and atmospheric NOM as well as extraterrestrial NOM have revealed remarkable structural variance which allowed detailed conclusions about their formation history. These in-depth molecular descriptions of NOM offer the opportunity to considerably improve the significance of future functional biodiversity studies which might lead to a novel, unified perception of biodiversity and biogeochemistry.

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