Computational Models of Dissolved Organic Matter

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Dissolved organic matter (DOM) plays a significant role in the biogeochemical processes of the aquatic and terrestrial environments including the global carbon cycle, microbial metabolism, transport of nutrients and contaminants. DOM is a complex heterogeneous mixture of several organic units. Molecular level interactions between those component molecules are responsible for active roles of DOM. Therefore, it is important to understand the behavior of DOM at the atomistic/molecular level. Here, molecular dynamics (MD) simulations were used to explore the interactions between the component molecules of DOM. Model lipid, peptide, carbohydrate, lignin, and low molecular weight organic compounds were simulated along with cations in water for 200ns. Various components of DOM aggregate to form dynamic supramolecules consisting of a hydrophobic core and an amphiphilic exterior. The molecular surface of DOM is composed of both hydrophobic and hydrophilic groups allowing DOM to bind with polar and non-polar molecules. DOM models for Leonardite humic acid and Suwanee River DOM were constructed and validated based on their elemental compositions and other available properties. The DOM models will be used to estimate the physiochemical properties for the biogeochemical reactions of DOM. Further refinement of the DOM models will involve increasing the variety of building block molecules.