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Exploring macroscopic properties of soil organic matter using modeling and molecular simulations

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Soil Organic Matter (SOM) is composed of a complex and heterogeneous mixture of organic compounds. It is of great importance to understand its molecular structure, the conformations and water accessibility, as well as the interfaces and reactivity of SOM with its surrounding. SOM extracts permitted for decades a systematic way of studying SOM via the use of standardized samples. We used such standardized samples of the International Humic Substances Society (IHSS) to computationally explore the properties of SOM.

We used the Vienna Soil Organic Matter Modeler 2 (VSOMM2; Escalona et al. (2021); https://somm.boku.ac.at/) to produce representative, condensed-phase, atomistic models of IHSS samples. This online tool ensures greater chemical diversity of the models and reproduces the carbon distribution or organic composition estimated by NMR. Generated atomistic models were subjected to molecular dynamics simulations. We characterized these systems in order to observe differences in their structure and dynamics.

Our results indicate the importance of carboxyl and aromatic groups in the molecular interactions, specifically for their interactions with cations and indirectly for their aggregation properties. We also investigated the sorption properties of these systems by calculating the free energy of absorption of inserting a water molecule to the system, which values were affected by the water content, compaction and phases of the organic matter.

These investigations help improve our understanding of properties and behavior of soil organic matter at a molecular level that is not attainable to experiments. We hope that such studies will have a great impact on basic research involving SOM.