Molecular characteristics, proton dissociation properties, and metal binding properties of soil organic matter: A theoretical study

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Soil organic matter (SOM) is a key soil component involved in the carbon sequestration, plant growth and nutrient transportation, and sorption of contaminants such as heavy metals. SOM is highly heterogeneous and the various origin sources and different surrounding environments increase its complexity. SOM has been extensively studied in terms of its structure and properties based on chemical experiments and analytical techniques, but rarely at the molecular level.

We have developed an *a priori* method to predict the molecular properties of SOM, which incorporated computational molecular modelling, SPARC Performs Automated Reasoning in Chemistry's (SPARC's) chemical reactivity models, and linear free energy relationships (LFERs) [1]. Specifically, the method used SOM models simulated by molecular dynamics modeling based on the experimental elemental composition and functional group information of SOM. The molecular characteristics of the SOM molecules were calculated including the molecular H/C and O/C ratios, molecular weight, aromatic index, and double bond equivalence. For the proton binding constants, SPARC calculated the microscopic pK_a values of every binding sites of individual molecules of the SOM model. Based on the pK_a values, the metal binding constants for individual monodentate binding sites were calculated using the Irving-Rossotti LFERs for different heavy metals. The results agreed reasonably with the default values used in the Windermere Humic Aqueous Model (WHAM) (VI). The theoretical SOM models, to some extent, represented the average properties of the investigated SOM. Overall, our study gives new quantitative and molecular insight into the structure and chemical properties of SOM. Such feasible and straightforward predictive scheme is useful to assess the risk of heavy metals in various aquatic and terrestrial environment involving heterogeneous natural organic matter.

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