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Unified Modeling Approach for Quantifying the Proton and Metal Binding Ability of Soil Dissolved Organic Matter

QIANTING YE, YANG DING, ZECONG DING, RONG LI AND ZHENQING SHI

South China University of Technology

Presenting Author: esyqt2020@mail.scut.edu.cn

Soil dissolved organic matter (DOM) is composed of a mass of complex organic compounds in soil solutions and significantly affects a range of (bio)geochemical processes in soil environment. Among the chemical reactivities of DOM (e.g., redox, photochemical activity, proton and metal binding, etc.), the proton and metal binding ability is one of the key properties controlling the fate of metals, which is highly related to the distribution of its heterogeneous binding sites of DOM molecules[1,2]. However, how the chemical complexity (i.e., heterogeneity and chemodiversity) of soil DOM molecules affects their proton and metal binding ability remains unclear, which limits our ability for predicting the environmental behavior of DOM and metals.

In this study, we specifically investigated the roles of the molecular diversity of a total of 24 soil DOM in regulating the proton and copper (Cu) binding ability of DOM molecules. Furthermore, a unified theoretical modeling approach, which combined FT-ICR-MS data, statistical analysis, and molecular modeling with VSOMM, for the first time, was developed for quantifying the proton and metal binding ability of diverse soil DOM according to the molecular properties of representative molecular groups[3]. One key novel finding of this research is that, despite the diverse chemical properties of different soil DOM, the molecules of all soil DOM can still be divided into three representative groups, and, based on the molecular models for individual molecular groups, we were able to further develop molecular models for all soil DOM to predict their proton and metal binding ability. This may be a new and feasible way to simplify the complexity of DOM and reduce the uncertainties of molecular models, but still to provide accurate representation of molecular properties. We expect that our modeling results will help to develop mechanistic models for predicting the reactivity of soil DOM from various sources.

[1] Zhenqing Shi, et al. (2016) *Environ. Sci. Technol.* 50, 10476-10484.

[2] Qianting Ye, et al. (2022) *Sci. Total Environ.* 843, 156996.

[3] Qianting Ye, et al. (2023) *Environ. Sci. Technol.* 57, 831-841.