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Molecular dynamics simulations of the interaction dynamics of labile organic biomolecules at a clay-water interface

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The selective adsorption of organic biomolecules on clay minerals play an important role in the formation and persistence of soil organic matter (SOM). Multiple interaction mechanisms (such as electrostatic interactions, H-bonding, water bridging, and cation bridging) were proposed to be responsible for the adsorption behavior of structurally different biomolecules. However, the relative contributions of these interaction mechanisms have not yet been explored. Here, using molecular dynamics simulations of a fully hydrated system, we monitor dynamic interactions during the adsorption path of ten structurally different organic compounds on montmorillonite, a smectite clay. Using algorithms developed in our lab to analyze each frame during the dynamics run, we tracked both the center of mass of each compound from the bulk solution to the mineral surface and the contribution of multiple adsorption mechanisms at the mineral surface. We found that (1) the relative contribution of each adsorption mechanism was variable across the adsorption dynamics time; (2) reversible adsorption occurred for all compounds on the clay surface even when strong interactions did occur during the simulation run; (3) total retention time of organic compounds near the clay surface did not correlate positively with its adsorption affinity observed experimentally (**Fig 1**). These findings provide new mechanistic insights into the dynamic adsorption of structurally different organic compounds in clay-organic formations.

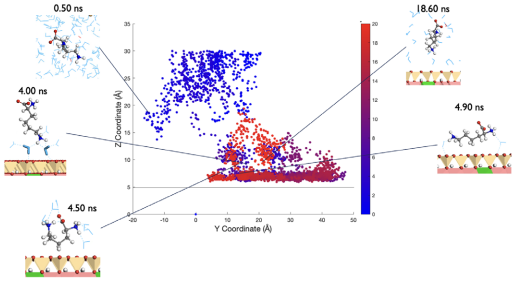

Figure 1: Dynamic trajectory of lysine relative to the water-clay interface. The scattered plot illustrates the paths of the center of mass of the lysine adsorptive at each time frame during the 20-ns dynamic run. The color baron the right side represents the simulation time for the scattered plot: 0 ns (dark blue), 10 ns (purple), 20 ns (red). The horizontal line at z = 5 Å represents the clay basal surface.