

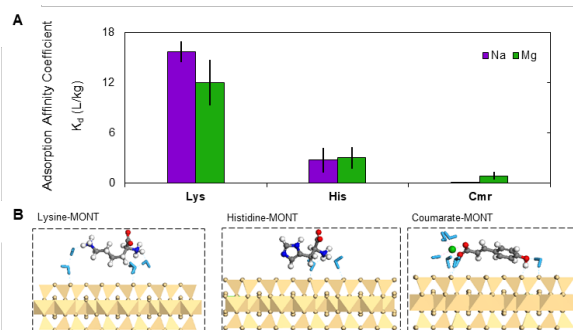
# Adsorption of structurally different organic biomolecules at water-clay interfaces

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As the largest terrestrial pool of organic carbon, soil organic matter (SOM) plays an important role in the global carbon cycle. Critical to SOM stabilization is the formation of organo-clay complexes through selective adsorption of organic biomolecules derived from plants and microbes. However, much still remains unknown about the mechanisms underlying the adsorption selectivity of clay minerals for heterogeneous organic mixtures. Here, using montmorillonite as a clay mineral commonly found in soils, we investigated the single and competitive adsorption of ten structurally different organic molecules (7 amino acids, 2 sugars, and 1 lignin derivative) as model SOM precursors. Liquid-state nuclear magnetic resonance spectroscopy was used to quantify these compounds in solution. We found that (1) positively charged amino acids had the highest adsorption affinity for the clay surface; (2) divalent metal cations in solution inhibited the adsorption of these positively charged compounds but facilitated the adsorption of negatively charged compounds such as lignin derivatives (**Fig. 1A**); (3) competitive adsorption occurred amongst favorable adsorptives in the presence of divalent metal cations. Intercalation of organic compounds in the clay interlayers was examined by X-ray diffraction. Using molecular modeling simulations of the different adsorbate conformations (**Fig. 1B**), we quantified the contributions of the various adsorption mechanisms (electrostatic interaction, H-bonding, water bridging, and cation bridging) that mediate the adsorption selectivity observed experimentally. This study lays a mechanistic foundation for understanding the hierarchical interactions of diverse soil organic compounds with clay minerals.



**Figure 1. Comparison of adsorption affinity and adsorbate conformations.** (A) Adsorption affinity coefficients for lysine (Lys), histidine (His) and p-coumarate (Cmr) adsorption to montmorillonite (MONT) in NaCl or MgCl<sub>2</sub> solutions (ionic strength = 0.15 M). (B) Molecular modeling of adsorbate conformations of Lys, His and Cmr on the clay (montmorillonite, MONT). Color code for b: hydrogen-white, oxygen-red, nitrogen-blue, carbon-grey, magnesium-green, water-light blue, MONT-light yellow.