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Competitive adsorption of labile biomolecules at water-iron oxide interfaces

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In sediment and soil environments, adsorption of labile biomolecules onto iron oxide is critical for the preservation of organic matter by limiting the mobility and bioaccessibility of adsorbed compounds [1]. The coexistence of diverse biomolecules may lead to competitive adsorption, thus influencing the binding dynamics of these labile biomolecules [2]. Here, to gain insights into the competitive adsorption of biomolecules, we reacted ferrihydrite, a low-crystallinity iron oxide, with a mixture of seven biomolecules including one nucleotide, one sugar, one lignin derivative, and four amino acids. Liquid-state nuclear magnetic resonance spectroscopy was used to quantify these biomolecules in solution. Our adsorption data revealed that compared to neutral biomolecules, biomolecules with either positive or negative charges have significantly higher adsorption on ferrihydrite (**Fig.1A**). Notably, the adsorption of nucleotide adenosine monophosphate (AMP), which was the highest in single-adsorptive scenarios, inhibited the binding of other biomolecules consistently (**Fig.1A**). We performed molecular modeling simulations to predict the conformations of adsorbed biomolecules and revealed the interaction mechanisms (**Fig.1B**). Our findings provide mechanistic insights into the binding dynamics of biomolecules on iron oxides.

[1] Faust, J. C., Tessin, A., Fisher, B. J., Zindorf, M., Papadaki, S., Hendry, K. R., ... & März, C. (2021). Millennial scale persistence of organic carbon bound to iron in Arctic marine sediments. *Nature Communications*, *12*(1), 275.

[2] Swenson, T. L., Bowen, B. P., Nico, P. S., & Northen, T. R. (2015). Competitive sorption of microbial metabolites on an iron oxide mineral. *Soil Biology and Biochemistry*, *90*, 34-41.

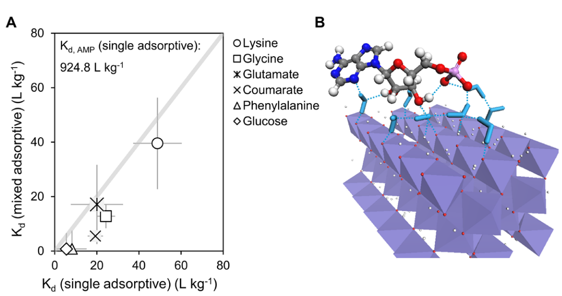

Figure 1. Adsorption affinity and adsorbate conformation of biomolecules on ferrihydrite. (A) Comparison of adsorption affinities of the biomolecules from single- and mixed-compound solutions reacted with ferrihydrite. (B) Adsorbate conformation of adenosine monophosphate predicted from molecular modeling simulations. Color scheme for atoms in (B): C (gray), H (white), O (red), N (dark blue), P (pink), Fe (purple), and atoms in water (blue). In (B), dashed blue lines indicate hydrogen bonds with criteria of 2.5 Å for the maximum distance and 120° for the minimum angle between the hydrogen bond donor and acceptor. Only water molecules involved in water-bridged hydrogen bonds between the biomolecule and ferrihydrite surface are shown; all other water molecules in the hydrated adsorbate conformation are removed for clarity.