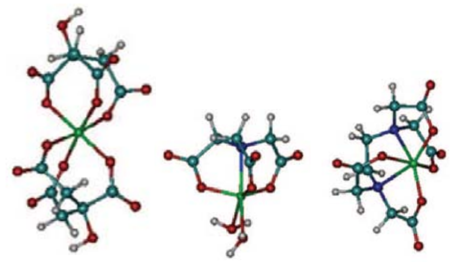
Metals with a Complex

Better bioremediation through metal-ligand complex studies

New details about how bacteria and metals interact highlight the importance of considering metal-ligand complexes as part of bioremediation strategies. Bacteria such as *Shewanella oneidensis* MR-1 hold promise as a bioremediation tool because they exchange electrons with metals, affecting their solubility and thus their level of danger to the environment and human health. As part of the Biochemistry Grand Challenge sponsored by the Department of Energy's EMSL, scientists have made significant progress toward understanding electron exchange between bacteria and metals. The research team led by the Pacific Northwest National Laboratory carried this Grand Challenge further by using spectroscopy and computational tools at EMSL to determine the kinetics of electron exchange when the metal, iron, is coupled to ligands of geological and environmental significance.



Computed structures of Fe-(citrate)$_2^{3-}$ (left), FeOH-NTA$^-$ (middle), and Fe-EDTA$^-$ (right).

In particular, the research team determined how Fe(III) complexes with the ligands citrate, nitrilotriacetic acid (NTA), and ethylenediaminetetraacetic acid (EDTA) were reduced by two *Shewanella* surface proteins known to be involved in electron transfer: MtrC and OmcA. The team's results were surprising: even though electron transfer from the surface proteins to the Fe(III) EDTA complex is thermodynamically unfavorable compared to reactions involving Fe(III)-citrate and Fe(III)-NTA, it happened most quickly. For the EDTA reactions, the reaction rate was influenced by the relatively large reorganization energies of the reactants – so much so as to override the strong thermodynamics. This and the geometry of the molecules in the reactions favored the electron transfer kinetics involving EDTA. The team's work demonstrates the importance of metal complexation to bioremediation. For contaminated sediments where radioactive metals are co-disposed with organic chelating agents, any effective bioremediation strategy should take into consideration the ligand complexation effect.

Scientific Impact: Experimental and computational studies such as these refine the understanding of the fundamental biological process of bacterial electron transfer and contribute to EMSL's goal to rapidly link theory and experiment. Further, such studies contribute heavily to EMSL's Biochemistry Grand Challenge.

Societal Impact: The team's work may lead to enhanced bioremediation strategies to remedy contaminated environments, such as the DOE's Hanford Site in Richland, Washington.

For more information, contact EMSL Communications Manager Mary Ann Showalter (509-371-6017).

Reference: Wang Z, L Shi, C Liu, X Wang, MJ Marshall, JM Zachara, KM Rosso, M Dupuis, JK Fredrickson, and SM Heald. 2008. "Kinetics of Reduction of Fe(III) Complexes by Outer Membrane Cytochromes MtrC and OmcA of *Shewanella oneidensis* MR-1." *Applied and Environmental Microbiology* 74(21):6746–6755.

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