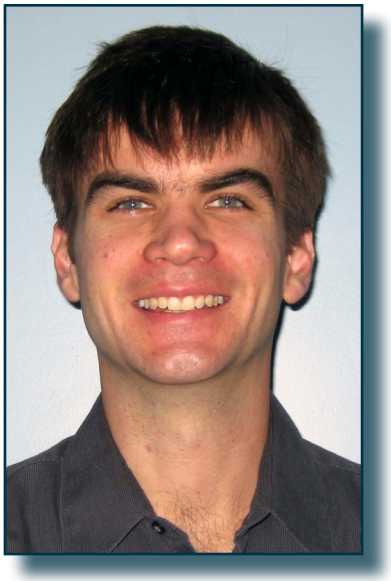
University of Minnesota
Driven to Discover℠

Department of Chemistry

Seminar

9:45 a.m. Tuesday, January 18 • 331 Smith Hall



National Institute of Health National Research Service Award
Postdoctoral Research Fellow

Matthew Liptak, Ph.D.

University of Rochester, Rochester, N.Y.

Diverse Functions of Metal Tetrapyrroles in Biological Systems: Investigating How the Protein Active Site Tunes the Electronic Structure

Abstract

The combination of spectroscopy and electronic structure calculations has provided exciting insights into the properties and functions of two metal tetrapyrrole-containing proteins, cobalamin-dependent methionine synthase (MetH) and cytochrome (cyt) c. Comparison of the magnetic circular dichroism (MCD) and electron paramagnetic resonance (EPR) spectra of MetH-bound cobalamin to those of the enzyme-free cofactor revealed that the protein environment perturbs the electronic structure of the cobalamin cofactor. When interpreted within the framework of density functional theory (DFT) calculations, these studies uncovered details regarding the MetH cofactor activation mechanism. While MCD and EPR spectroscopies are sensitive probes of transition metal centers, nuclear magnetic resonance (NMR) spectroscopy is a superior tool for investigating both the tetrapyrrole ligand and the polypeptide environment. To date, interpretation of the NMR spectra of paramagnetic metalloproteins has been limited by the lack of an interpretive model rooted in modern electronic structure theory calculations. This talk will discuss the implementation of such a model and its application to cyt c. These combined NMR and DFT studies of paramagnetic cyt c have clarified determinants of the heme reduction potential and uncovered intriguing electronic structure changes in a human cyt c variant with increased apoptotic activity.

Host: Professor Christopher Cramer
Refreshments will be served prior to the seminar.