



## Pr Vincent PECORARO

Department of chemistry, University of Michigan  
[vlpec@umich.edu](mailto:vlpec@umich.edu)

# De Novo Metalloprotein Design: From Zn Hydrolytic Enzymes to Models of Mononuclear Cu Systems.

De Novo protein design provides an attractive approach for modeling the active sites of metalloproteins. Using this technique one may not only provide a synthetic construct which precisely mimics the first coordination sphere of a known metalloenzyme site, one may also develop a catalytic center that is embedded within a hydrophobic protein pocket and which has its coordination chemistry influenced by second coordination sphere ligands. In this presentation, we will discuss how to prepare a mixed Hg(II),Zn(II) protein that is capable of efficient, multiturnover hydrolysis of nitrophenylacetate in aqueous solution over the pH range 7.5 to 9.5. We also show this construct is capable of CO<sub>2</sub> hydration. The Zn(II) catalytic center is structurally homologous with those found in carbonic anhydrases and matrix metalloproteinases. We will also demonstrate how a structural site, in this case Hg(II), stabilizes the protein and leads to slightly enhanced catalytic activity. Recently, we have been able to prepare structural models for CuN<sub>3</sub>O systems such as nitrite reductase. We will show how Cu(I) binds to our peptides and is capable of complexing CO into the hydrophobic protein core. Finally, we will discuss direct reactions of this designed peptide with nitrite, demonstrating nitrite reductase activity for this system.

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15 rue Hélène Brion, 75013 Paris

Contact : Elodie Anxolabéhère-Mallard  
 Université Paris Diderot, UFR de Chimie

Tél: 33 0 (0) 1 57 27 87 84 – [elodie.anxolabehere@univ-paris-diderot.fr](mailto:elodie.anxolabehere@univ-paris-diderot.fr)