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

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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. Furthermore, this new catalyst carries out CO₂ hydration better than any previously characterized biomimetic system. The Zn(II) catalytic center is structurally homologous with those found in carbonic anhydrases and matrix metalloproteinases. Recently, we have been able to prepare structural models for Type 2 copper environments such as found in nitrite reductase. We will show how Cu (I) binds to our peptides in a CuN₃O coordination geometry and is capable of complexing CO into the hydrophobic protein core. Most important, this designed copper protein is redox active and can convert NO₂⁻ into NO and H₂O, thus serving as a reactivity mimic for nitrite reductase activity.

sala de Graus de la Facultat de Ciències, 12h

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