World Academy of Science, Engineering and Technology
International Journal of Bioengineering and Life Sciences
Vol:15, No:08, 2021

De Novo Design of a Minimal Catalytic Di-Nickel Peptide Capable of Sustained Hydrogen Evolution

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Abstract : On the early Earth, protein-metal complexes likely harvested energy from a reduced environment. These complexes would have been precursors to the metabolic enzymes of ancient organisms. Hydrogenase is an essential enzyme in most anaerobic organisms for the reduction and oxidation of hydrogen in the environment and is likely one of the earliest evolved enzymes. To attempt to reinvent a precursor to modern hydrogenase, we computationally designed a short thirteen amino acid peptide that binds the often-required catalytic transition metal Nickel in hydrogenase. This simple complex can achieve hundreds of hydrogen evolution cycles using light energy in a broad range of temperature and pH. Biophysical and structural investigations strongly indicate the peptide forms a di-nickel active site analogous to Acetyl-CoA synthase, an ancient protein central to carbon reduction in the Wood-Ljungdahl pathway and capable of hydrogen evolution. This work demonstrates that prior to the complex evolution of multidomain enzymes, early peptide-metal complexes could have catalyzed energy transfer from the environment on the early Earth and enabled the evolution of modern metabolism

Keywords : hydrogenase, prebiotic enzyme, metalloenzyme, computational design
Conference Title : ICALR 2021 : International Conference on Astrobiology and Life Research
Conference Location : Vancouver, Canada
Conference Dates : August 05-06, 2021