SMART Teams 2014-2015 Research and Design Phase

Laconia High School SMART Team

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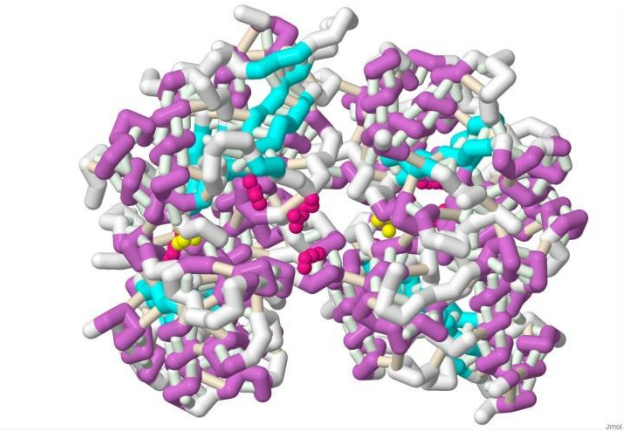
[FeFe] Hydrogenase in Artificial Photosynthesis

PDB: 3XL4

Primary Citation: Muleder, David W., Eric S., Boyd, Ranjuana Sarma, Rachel K. Lange, James A. Endrizzi, Joan B. Broderick, and John W. Peters. "Stepwixe [FeFe]-hydrogenase H-cluster Assemly Revealed in the Structure of HydA." *Nature* 465 (2010): 248-51

Format: Alpha carbon backbone

RP: Zcorp with plaster



Description:
The development of clean and renewable energy is critical to partially address the energy crisis and climate issues. Inspired by nature, artificial photosynthesis through water splitting by solar energy conversion is the most attractive approach for the development. The overall water splitting includes two half-catalytic reactions, i. e. hydrogen (HER) and oxygen (OER) evolution reactions. An efficient catalyst is required to perform each of these catalytic reactions. Molecular catalysts that mimic the function of [FeFe] hydrogenase are among the most effective synthetic transition metal complexes known for HER. The Laconia SMART (Students Modeling A Research Topic) Team used 3D printing technology to model the active site of [FeFe] hydrogenase and understand its catalytic function for HER. [FeFe] hydrogenase is an enzyme that catalyzes proton reduction to bind hydrogen together. Arg265, Lys288, and Lys409 are positively charged residues that line the channel entrance. Lys 188 is at the end of the channel and may help to orient the 2Fe subcluster during hydrogen insertion. The fundamental understanding of the catalytic function of the [FeFe] hydrogenase active site in HER will provide insight into the rational design of efficient catalysts for solar fuel generation. The SMART Team program is supported by a grant from NIH-CTSA.

Specific Model Information:

- Backbone is colored white.
- Alpha helix is colored orchid.
- Beta sheets are colored aqua.
- Iron is colored yellow.
- Hydrogen bonds are colored honey dew.
- Amino acid side chains involved in the active site displayed in spacefill are colored deep pink.
    - Arg 275
    - Lys 288
    - Lys 409
    - Lys 188

http://cbm.msoe.edu/smartTeams/index.php

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