Westosha Central High School SMART Team

Authors: John Dietz, Brett Niederer, Trevor Millhouse, Connor Muff, Joyce Riphagen, Victoria Salerno, Elizabeth Van Kammen

Teacher: Jonathan Kao

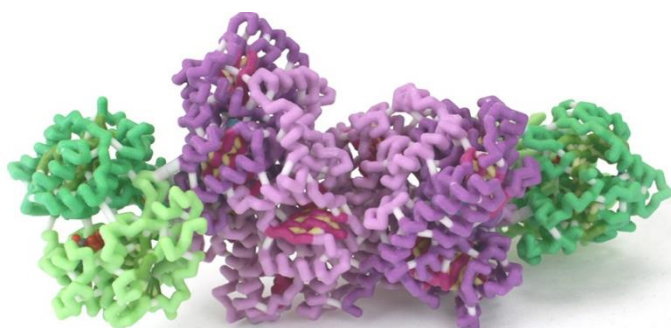Mentor: Edwin Antony, Ph.D., Marquette University

Getting N_2 Sustainable Fertilizer Production: Nitrogenase

PDB: 2AFI

Primary Citation: Tezcan, FA., Kaiser, JT., Mustafi D., Walton WY., Howard JB., Rees DC. (2005) Nitrogenase complexes: multiple docking sites for a nucleotide switch protein. *Science* 309(5739):1377-80

Format: Alpha carbon backbone

RP: Zcorp with plaster

Description: Fertilizer is an essential component of agriculture globally that is artificially produced through the Haber-Bosch process. This process requires energy to generate temperatures of 400-500 ^{o}C and pressures of 15-25 MPa to reduce N_2 to NH_3. The greenhouse gas CO_2 is produced as waste in this reaction. In nature, bacteria in plant root nodules reduce N_2 into NH_3 catalyzed by nitrogenase. Nitrogenase is a complex comprised of two proteins: a heterotetrameric MoFe protein, and two heterodimeric Fe proteins bound on each end. The MoFe proteins consists of two 491 residue α-subunits and two 522 residue β-subunits. The Fe proteins are bound to the exterior of the MoFe protein creating two mirrored functional halves. In an ATP facilitated process, the Fe protein captures an electron using an iron metallocluster, then donates an electron to the molybdenum/iron metallocluster in the MoFe protein. Electrons are moved within the MoFe protein to the active site. The two halves of the protein alternate in a coordinated manner, transferring one electron at a time until eight electrons are transferred. The electrons then reduce the N_2 substrate into $2(NH_3)$+ H_2. The Westosha Central SMART (Students Modeling a Research Topic) Team has created a 3D model of nitrogenase highlighting the metalloclusters and how the complex assembles/disassembles. Understanding how this protein functions may allow mass production of ammonia through a biological process reducing the dependency on the Haber-Bosch process therefore reducing CO_2 emissions.

Specific Model Information:

Beta Sheets in MoFe protein- medium violet red
Beta Sheets in Fe protein - olivedrab
Hbonds - pale golden rod
Struts - white

Fe Protein -
- E and G chains medium sea green
- H and F chains pale green

MoFe Protein -
- A and C chains medium orchid
- B and D chains are plum

SF4 Metallocluster - orange
CFN Metallocluster - cyan
CLF Metallocluster - gold
ADP – cpk

Ligands -
SF4 - electron donor in the Fe protein
CLF - electron acceptor in the MoFe protein
ICS - continues to move electron to the active site

> ADP - hydrolysis of ATP provides energy for the FE protein to capture/donate electrons. ADP is the resultant molecule

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