Westosha Central High School SMART Team

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Getting N_2 Sustainable Fertilizer Production: Nitrogenase

PDB File: 2AFI

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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.

Fertilizer is an essential component of agriculture globally. The world's fertilizer supply is artificially produced through the Haber-Bosch process. This process requires sufficient fossil fuels 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 found in plant root nodules reduce N_2 into NH_3 catalyzed by a protein called nitrogenase. Nitrogenase is composed of two functional halves that are mirror images of each other. In each half there is an exterior Fe protein, a heterodimeric electron donor containing an iron metallocluster, and an interior MoFe protein, a heterodimeric electron acceptor containing a molybdenum/iron metallocluster. In an ATP facilitated process, the Fe protein captures then donates an electron to the MoFe protein. Electrons are moved within the MoFe protein to the active site. Each cycle moves one electron to the active site therefore the protein requires multiple cycles to complete the chemical reaction. After accumulating eight electrons, the N_2 substrate is reduced into $2(NH_3)+ H_2$. The two halves of the protein alternate in a coordinated manner, transferring one electron at a time. 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 for creating fertilizer while reducing CO_2 emissions.

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Audubon Feedback

Peer Review Comment Sheet
(Send to the SMART Team and to Judy)

Clarity

1. What is the "big picture" or "hook" of this project?
-Fertilizer is an essential component of agriculture globally. OR The world's supply of fertilizer is artificially produced through the Haber-Bosch process where atmospheric nitrogen is separated through intense heat and pressure.
- Try to more be more clear, unclear which one is the hook.

2. What is the specific molecule that has been modeled and what is its normal function within the cell?
-Nitrogenase
-It captures and donates an electron to the MoFe protein

3. What is the connection between the "big picture" and the specific protein modeled?
-Fertilizer is essential to agriculture globally
-4% of world's energy is used
-Increase in global food production
-Reduce CO_2 emissions

4. What are specific structural features that are important to the function of this protein?
-not found

Checklist for Abstract Format
Please check below if the feature was addressed in the abstract:

___ ☐____ The abst
printing technology.

___ ☐____ The abstra
Team advisor and SMART Team mentor.

___ ☐bstract The abstract was concise and meets the 1720 character count criterion.

___ ☐____ The abstract p
picture.

Additional Comments:
If you have any additional suggestions for improvement upon the abstract, please indicate those in this section.
-Title isn't super interesting

-You need to include your school name and say what you are modeling and how you are modeling it
-Nothing about structure- Ex: Alpha Helix and Beta Sheets,
-Pick either the energy usage or the reduced CO_2 emissions to focus on for benefits of your molecule
-a transition could be used to tie the hook to the protein you are modeling
-Middle section about how the protein works is written well
-more about MoFe protein

- Nitrogenase
    - Big Picture
        - Manufacture fertilizer
        - ammonia - based / manufactured via Haber - Bosch process
        - Bacteria fix nitrogen naturally using a complex of proteins
            - “Nitrogenase”
    - Structure
        - Complex of protein composed of a mirror image of Fe + MoFe
        - Fe and MoFe proteins
        - Fe (electron donor) uses ATP in order to get electrons to MoFe (electron acceptor)
        - Electrons go to active site where N_2 is broken down into NH_3+H_2 using 8 electrons