



SMART Teams 2013-2014

Research and Design Phase

Brown Deer High School SMART Team

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Myoglobin: O₂ or Not O₂ . . . That is the Question.

PDB: 2MGK

Primary Citation: Quilllin, M.L., Arduini, R.M., Olson, J.S., Phillips Jr., G.N. (1993). High-resolution crystal structures of distal histidine mutants of sperm whale myoglobin. *Journal of Molecular Biology* 234: 140-155.

Format: Alpha carbon backbone

RP: Zcorp with plaster

Description:

Free divers can't hold their breath as long as whales, but they train their bodies to maximize their oxygen (O₂) storing potential using the protein myoglobin. Myoglobin's structure has been known for decades, but researchers are still trying to determine just how myoglobin functions. Found in muscle tissue, myoglobin stores O₂, a molecule needed to produce chemical energy. Toxic ligands, such as carbon monoxide (CO) and cyanide, also bind to myoglobin. When CO binds to a free heme group, the heme's binding affinity for CO is 20,000 times that for O₂. When heme is surrounded by myoglobin, that binding affinity ratio drops to only 25. The decrease was thought to be due to steric interactions which prevented CO from occupying the same space as His64. Recent evidence suggests that electrostatic interactions and hydrogen bonds play a more important role. The O₂ is stabilized as opposed to the CO being pushed out. Several amino acids (His64, Val68, Phe43, Phe46, and Leu29,) seem to stabilize the ligand. With 3D printing technology, the Brown Deer SMART (Students Modeling a Research Topic) Team, funded by a grant from NIH-CTSA, created a model of myoglobin. If researchers can fully understand ligand discrimination by heme proteins, not only will divers be able to hold their breath longer, but we may be able to cure diseases like anemia where there is a lack of O₂ in the blood.



Specific Model Information:

- Alpha helices are highlighted in orange.
- The alpha carbon backbone is colored honeydew.
- The heme group is displayed in ball and stick and colored in cpk.
- Carbon monoxide is displayed in ball and stick and colored in cpk.
- Amino acids (Leu29, Phe43, Phe46, His 64, Val68 and His93) responsible for stabilizing the ligand are displayed in ball and stick and colored in cpk.
- Amino acids (Gly, Leu and Gln), displayed in ball and stick and colored in cpk, are swappable with His64.
- Structural supports are colored peach puff.

<http://cbm.msoe.edu/smartTeams/>

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