



SMART Teams 2013-2014

Research and Design Phase

Whitefish Bay High School SMART Team

Sam Broadnax, Jieun Heo, John Schroeder, Michelle Shin, Frank Zhang, Nick Longo, Brianna Donaldson Morton, Jamelah Johnson, Morgan Phillips, Brenna Grych, Koobmeej Xiong, Ryan Davis, Laura Prekosovich, Camille Middleton, Tony Cho, Grant Von Paumgarten, Philip Flejsierowicz and Jon Ebert

Teachers: Katie Brown and Paula Krukar

Mentors: Dmitry G. Khomyakov, Ph.D. Candidate and Qadir K. Timerghazin, Ph.D.,
Marquette University Chemistry Department

NO S-nitrosylation, NO Memorization

PDB: 2DGV

Primary Citation: Abe, C., Muto, Y., Inoue, M., Kigawa, T., Terada, T., Shirouzu, M., Yokoyama, S.
Solution structure of the RNA binding domain in Heterogeneous nuclear ribonucleoprotein M. To be published.

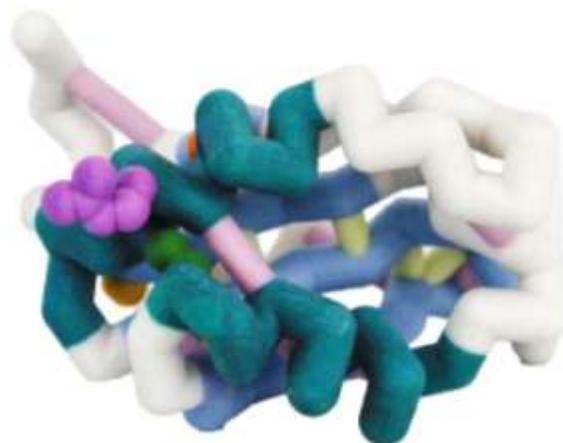
Format: Alpha carbon backbone

RP: Zcorp with plaster

Description:

Nitrogen and oxygen are two components of the air we breathe.

Bonded together as nitric oxide, they are an important signaling molecule that is involved in numerous physiological processes including the protein S-nitrosylation. The human body cannot function without this effective process, but if the regulation of this process breaks down, it can lead to common diseases such as Parkinson's and Alzheimer's. Irregular nitrosylase and denitrosylase activities may be involved in these diseases, so they are important therapeutic targets. This important process also allows blood vessels to expand, so they can transport more blood and retain more oxygen. The key component, nitric oxide (NO), attaches to glutathione to give the S-nitrosoglutathione molecule (GSNO). The NO from the GSNO then travels to a specific cysteine in a protein, which can affect the properties of that protein. Using 3D printing technology, the Whitefish Bay SMART (Students Modeling A Research Topic) Team is aiding its mentors as they research to figure out why the NO attaches to one cysteine specifically and what exactly this process does. Doctor Timerghazin and Dmitry G. Khomyakov hypothesize that a positive amino acid, such as arginine, catalyzes the NO transfer and causes it to jump to the specific cysteine. Discovering what S-nitrosylation's physiological role as well as why one cysteine is chosen over others could lead to developments in our understanding of certain diseases that are linked to the erratic regulations of S-nitrosylation in the human body.



Specific Model Information:

- Non-motif sections of the alpha carbon backbone are colored white.
- Alpha helices are highlighted in light sky blue.
- Beta sheets are highlighted in teal.
- Amino acid Cys675, displayed in ball and stick and colored green, is active in the S-nitrosylation process.
- Amino acids Cys652, Arg706 and Cys708, displayed in ball and stick and colored yellow, dark purple and orange respectively, are potential factors in the S-nitrosylation process.
- Hydrogen bonds within the beta sheets are colored cream.
- Structural supports to stabilize the model are colored light purple.

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

The SMART Team Program is supported by the National Center for Advancing Translational Sciences, National Institutes of Health, through Grant Number 8UL1TR000055. Its contents are solely the responsibility of the authors and do not necessarily represent the official views of the NIH.