Assignment #7: Data Mining & Molecular Modeling of Biological Sensing Protein

It is the goal of Assignment #7 to explore and analyze structure-function relationships of biological indicators / sensors. Select a biological sensing protein from the Protein Data Bank, read the primary literature to learn about the role of the selected sensor in its biological context, and learn how to employ molecular modeling to support your learning / understanding / discussion of the chemical mechanisms of the sensing events.

(a) Select Biological Sensing Protein. The Protein Data Bank is located at http://www.rcsb.org/ and a link is provided on the assignment page of the course web site. Focus your PDB search on the crystal structures of the following sensing proteins: (1) Green Fluorescent Protein GFP (206 Hits!), (2) Calcium Ion Sensing Protein (34 Hits), (3) O_2-Sensing Protein (23 Hits), and (4) CO-Sensing Protein CooA (3 Hits). The selection of other topics is possible and can be considered in consultation with the instructor. Select the protein structure that you want to discuss. In one paragraph, justify your selection and explain the role of this sensor in its biological context with proper citation of primary sources.

(b) Analyze the Sensing Protein. Using the online tools provided by the PDB portal, locate the active site of the protein and analyze the immediate neighborhood of its active site. Arrange the display such that the pertinent features of the active site can be viewed well, and create one image of the display. You can use several images if that is necessary for a proper appreciation of the active site. Show the image(s) in Figure 1 and include major structural parameters in the Figure caption (not too many, select thoughtfully). Write one paragraph to describe the protein's active site and any significant changes to the structure during the sensing event.

(c) Molecular Model the Sensing Event. Using the molecular modeling program Chem3D installed on departmental computers, build small models of the active site before and after the sensing event, optimize the 3D-structures of your models (minimize MM2 energy), create images of ball-and-stick, stick, and space-filling models, show these images in Figure 2 and

include major structural parameters in the Figure's caption. Write one paragraph to describe the models and explain the chemistry of the sensing event using these models for illustration.

"Major structural parameters" include the most characteristic bond lengths, angles and dihedrals. Such parameters usually describe the geometry of functional groups and they include especially any parameters that undergo change during the sensing event. Feel free to alter default settings for structure display (i.e., atom size, color, …) as you see fit.

Submission & Target Dates: The assignment must be completed using PDB software, CambridgeSoft modeling software ("Chem3D"), and MS Word with *JOC* formatting. Your submission should contain a title, three paragraphs, two Figures, and a properly formatted reference section. Submit one Word file "A07_'your name'.docx" by Tuesday, 03/22/11, midnight. Bring one hardcopy in color to class on Wednesday, 03/23/11, for peer-review.