

# Molecular Graphics Task Force

## Introduction

There is little doubt that the ability to visualize the structures of biomolecules on personal computers has vastly increased our ability to better study their structure-function relationships. Before the advent of PC friendly programs, only the “anointed few” were able to benefit from molecular graphics program operating on Evans and Sutherland or Silicon Graphics systems operating off of main frame computers. Presently there are a few web sites listed below that have outstanding Jmol routines that tell detailed stories about the listed proteins or complexes. However, there are **no** web sites that contain the number or cover the breadth of topics as does the Bioc 462a Molecular Graphics Gallery. The routines in this Gallery are designed to address a specific point being accentuated in the lecture format rather than attempting to tell a complete story about the proteins or molecules, therefore are not as detailed as other web sites.

## A Brief History

The use of molecular graphics in Bioc 462a and 462b began in the early 1990's by the late Professor Michael A. Wells, with help from Professor William Montfort and James Pennington, who felt that their usage would greatly improve student's understanding of the concepts being discussed in class. The routines that Dr. Wells developed were designed to be short and to the point enhancing the class room learning experience. Routines were developed using RasMol scripts that were incorporated into a web page program called Chime. Subsequent routines were added to the Bioc 462a gallery by Drs. Elizabeth Vierling, James Hazzard, Miriam Ziegler, and Thomas Baldwin. Chime was a laborious program to use and was ultimately abandoned. As RasMol began to be phased out the the program Jmol came upon the scene. Using Jmol, it became much easier to generate molecular graphics web pages, as the students in Bioc 463a have learned. In 2004, Dr. Hazzard, Daniel Martinez, and Aaron Miller (the latter two were undergraduates in Bioc 463a) converted all of the existing Chime routines into Jmol web pages. Subsequent additions were made by Drs. Baldwin and Zeigler who were teaching Bioc 462a.

## Purpose of the Task Force

The Bioc 462a Molecular Graphics Gallery has remained essentially unchanged since 2004. Quite often these routines were developed immediately before a lecture; therefore these routines were often minimalistic in their “artistry” and utilitarian in nature;

seldom, if ever, was the “WOW!” factor taken into consideration. Now that some of our talented undergraduates have learned about the processes involved in generating Jmol web pages and have seen these pages used in Bioc 462a, understanding the context in which they were employed, we would like to call upon their intellectual and artistic talents to begin the process of updating and improving the routines that are posted in Bioc 462a Molecular Graphics Gallery.

### **How to Get Involved**

Since this project involves modifying existing Jmol routines, a working knowledge of the process by which these routines are generated is an absolute requirement. A student who wishes to participate should contact Dr. Hazzard and sign up for Bioc 492, receiving 1 unit credit for your efforts. Then choose one routine, examine it critically, and decide what changes you would like to make to the routine to either clarify the story the routine is attempting to tell, or make it more artistic (i.e., improving the “WOW” factor), remembering the intended audience and purpose of the routine. After modifying the routine, the results need to be presented to Dr. Hazzard, who will upload the modified script to the web server.