

Qualification Phase

Task #4

Initial Qualification Model Jmol file & Design Sheet

Due: Friday, October 6th

1. **Design a model** of PDB File **3zmk** using Jmol version **14.15.3** and following the design specifications located in the next section. Attach the exported jpg file of your completed model design to an email to Judy (birschbach@msoe.edu).

Please use **Jmol 14.15.3**, which you can download from the CBM website: <http://cbm.msoe.edu/smartTeams/smartTeamsLocal.php>. This is a free program and should operate on both PCs and Macs. A Jmol Training Guide has been designed to help you in learning the commands in the Jmol program.

****PLEASE NOTE:** Jmol releases updated versions of Jmol on a regular basis through the Jmol website. For the purposes of SMART Team designs, please **ONLY USE Jmol 14.15.3** for your SMART Team 2017-2018 model designs.

2. **Thoroughly review the model using the Model Design Checklist** found after this task. Any unaddressed inappropriate model features will prevent your team from being checked off for this task.
3. Complete a **Model Design Sheet** (Use the chart found on page 3 of this task) and email this file to Judy. Your model design sheet will provide us with a description of your model. This chart is essential in case our model builders encounter any issues with your Jmol design, we will use this sheet as the guideline to understanding what you are trying to display.
4. ****Name** your .jpg file according to the following format when you attach your file and email it to Judy:

school name_protein abbrev_pdb id_ver#

Example: **Cudahy_GST_3zmk_ver1**

Model Design Specifications

1. PDB file: [3zmk.pdb](#)
2. [1.5 Alpha-carbon backbone](#) format should be displayed.
3. [Remove cartoon format and water molecules](#)
4. [Design values](#) (You must use these values):
 - a. Backbone 1.5
 - b. Bonds & Struts 1.0
 - c. Spacefill (sidechains) 1.25
 - d. Wireframe (sidechains) 1.0
5. [Add Hbonds to beta-sheets](#) only
6. Remove any “triangle” Hbonds from the beta-sheets
7. Add [struts](#) to create a stable physical model
8. Display the [sidechains](#) in Chlororoxin that play a significant role in the function of the protein. Remember to have a [clean backbone](#) with your sidechains.
9. When coloring sidechains, avoid coloring the backbone of the sidechain.
10. Remove any struts that skewer sidechains.
11. Display and attach with struts any [significant ligands](#) (1.25 spacefill & 1.0 wireframe) to the enzyme.

Helpful Tips

1. Colors: When you use color in your model design, we recommend that you make your selections carefully. **Do NOT use black**, because black does not print well. If you want to highlight a feature, chose a light color on a dark background OR a dark color on a light background.
2. Always select bright or contrasting colors to highlight significant features. Use neutral colors on less significant features such as hydrogen bonds or struts. If you would like to use multiple shades of the same color, choose shades that are distinct enough to be able to see a difference on the printed model.
3. A JavaScript color sheet has been provided to aid in deciding your color choices for highlighting the various aspects of your model. You may also refer to the website (<http://jmol.sourceforge.net/jscolors/>) for color choices

This task will be marked as complete on the progress bar when your team emails the Jmol jpg file **AND** the model design sheet to Judy (birschbach@msoe.edu) by

Friday, October 6th

First, second and third place WILL be awarded for Task #4!

School Name:	
Advisor Name(s):	
Protein Name:	Glutathione-S-Transferase
PDB File:	3zmk
Jpg filename:	<i>(school name_GST_3zmk_ver#)</i>
<u>Basic features</u> included (bonds, stuts, secondary structures, domains, etc) and their specific colors:	
<u>Amino acids</u> displayed and <u>WHY</u> (what role do these amino acids play in the structure & function of the protein).	
<u>Ligand(s)</u> displayed in your model and <u>WHY</u> are they important to the molecular story?	