**CHEM 132 Lab #8**

**Exploring Protein structure with the molecular visualization FirstGlance in Jmol**

*Instructions*

After completing these simple exercises, you should be familiar with how to use many of the basic commands in FirstGlance in Jmol.

These programs will allow you to manipulate protein and nucleic acid structures to suit your needs.

One note on color schemes. The CPK color scheme is commonly used in these exercises. In this convention, red = oxygen, blue = nitrogen, gray = carbon, white = hydrogen, and yellow = sulfur.

Follow these steps to access the macromolecular visualization program FirstGlance in Jmol.

**During each step you will need to capture the image and show it to your instructor.** An easy way to do this is to **take a screen-shot of the screen** by either Snip-it program (PC) or Grab-it program (mac). Your instructor will need to initial your lab for each screen-shot.

1. If you are using a **Mac** please use **Safari** as your web browser. Firefox may not run properly. If you are using a **PC** please use **Firefox** as your web browser. Chrome, Internet Explorer, and Microsoft Edge will all run much slower.

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2. Go to **http://bioinformatics.org/firstglance/fgij/**. This URL is the FirstGlance in Jmol web page. Enter **1LGD** in the PDB identification code window in the center of your screen. Hit **Submit.**

1LGD is protein with 261 amino acids. It is a protein involved in carbon dioxide transport and in the maintenance of pH in the blood. It has a simple compact structure that will make it a good place to learn to manipulate the images of macromolecules.

2. Your window will have 2 frames

The Structure Window- on Right

Control Menu- on Left (Top window with 4 tabs and bottom window)

3. Stop the molecule from spinning by un-checking the Spin button at the control menu on left

4. There are several ways that you can adjust what you are looking at and the instructions below will walk you through some of the manipulations. Anytime you want to reset the image, press the RESET in the control menu **Views** tab and the original file will reappear on your screen.

5. Now, let’s learn to rotate, zoom the molecule in the Structure window.

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | **MAC** | **PC** |
|  | ZOOM | Hold down the SHIFT key and the mouse button drag the mouse back and forth | Hold down the SHIFT key and the left mouse button drag the mouse back and forth |
|  | ROTATE | Hold down mouse button  move the mouse in a circular motion | Hold down the left mouse button  move the mouse in a circular motion |

You can also zoom in and out using the button in the control menu. Each time you press the button it will zoom an incremental amount.

6. There are 3 general ways to manipulate the image. They each have their merits so you will want to become familiar with each of them. These include:

a) Using the control menus under the **Views** tab (Left portion of the screen)

b) Typing into the command line (right click on structure, select **Console**: Open) – for this you will need to learn some of the syntax

c) Using the menu located in the structure window (right click on structure)

7. Let’s start with the **Views** tab within the control menu.

a) Select **Secondary Structure**. What secondary structure elements exist in the protein? Point out the N and C terminus. (Instructor initials\_\_\_\_\_\_)

b) Select **Composition.** What type of representation is this view? What color are the water molecules? Turn them off by clicking on the Water box in the control menu. If you turn them back on what is the new color of the water molecules? (Instructor initials\_\_\_\_\_\_)

c) Select **Hydrophobic/Polar**. From the structure can you say anything about the amino acid residues on the inside of the protein? On the outside of the protein? (Instructor initials\_\_\_\_\_\_)

d) Select **Charge.** How many positive residues are located on the outside of the protein?

(Instructor initials\_\_\_\_\_\_)

8. The protein is currently displayed in charged spacefillng mode. We can also display the charged space-filling mode by using the “right click” menu. First Reset. Place the cursor on the Structure window. Right click your mouse, Press **Select**-**All**. Right click your mouse again, click **Style**, **Scheme**, **CPK Space fill**.

9. The protein is currently displayed in charged space fill mode. Right click, **Select-All**. You can also change the display by using the command line (right click on the structure and select Console. A new console menu will open. Type: CPK off. Then hit return. It will now change to cartoon format. You may need to Type: Cartoon ON in order to see cartoon format (Buggy…..)

(Instructor initials\_\_\_\_\_\_)

10. You can also use the Jmole console to script other commands. For example if you wanted to color the helix blue. Type: select Helix, hit Return. Type: color cartoon blue. Hit Return.

(Instructor initials\_\_\_\_\_\_)

11. You can also pick out individual residues using the command line.

Type: select 47-51

Hit Return

Type: color cartoon red

Hit Return

(Instructor initials\_\_\_\_\_\_)

12. You can use both command lines in combination with the mouse. For example if you wanted to visualize a single amino acid in the helix.

Type: select 29

Hit Return.

Right click on structure, select Style, select Scheme and select Sticks

You can identify amino acid and all of its atoms by clicking on it. What amino acid is it?

(Instructor initials\_\_\_\_\_\_)

Type: select 40

Hit Return.

Right click on structure, select Style, select Scheme, and select Sticks

You can identify amino acid and all of its atoms by clicking on it. What amino acid is it?

(Instructor initials\_\_\_\_\_\_)

13. You can also measure the distance between any two atoms. To do this double click on the Nitrogen atom of the side chain residue 29. Drag your mouse over to the oxygen atom of the side chain of 40. This will give you the distance. Double click to fix the distance. (Instructor initials\_\_\_\_\_\_)

14. You can also select residues using the control menu.

Click on Find.

In the menu box below type in 53. Click on the residue, what amino acid is it?

Right click on structure, select Style, then select Scheme, then select Sticks

Clear the find box and type in 10. Click on the highlighted residue. What amino acid is it? (Instructor initials\_\_\_\_\_\_)

Right click on structure, select Style, select Scheme, select Sticks

Determine the distance between any of the atoms in side chain 53 to any of the atoms to side chain 10. (Instructor initials\_\_\_\_\_\_)

15. Use this tutorial to get more familiar with the program.

One thing to note is that there is currently no “UNDO” button. If you are not sure if you have selected the item of interest, simply change its color. That is easy to undo by changing it back to its original state. Reset

You will have to use the program more to learn all of its nuances. But this quick run through should get you started. Additional tutorials are available on-line. Jmol documentation site (<http://jmol.sourceforge.net/docs/>) and (<http://molvis.sdsc.edu/fgij/about.htm>).

1LGD does have a substrate(s) bound. To take advantage of this feature when exploring the structure of a protein you can use the control menu and click on/off Ligands+.

16. Another powerful feature is the Contacts & Non Covalent Interactions feature found in the **Tools** tab in the control menu.

Reset your protein and stop in from spinning. (Click Reset and then click Spin off)

Click on Contacts & Non Covalent Interactions

Change the view back and forth from Spacefill to Cartoon from **Views** tab in control menu. Observe the difference.

Select Residues/Groups from **Views** tab in control menu.

Select the ligand by clicking on it with your mouse on the structure. (It will appear with “\*” marks on it.)

Then click on **Show Atoms Contacting Target** (Instructor initials\_\_\_\_\_\_)

There are four different contact views. Click on each of them to visualize their differences. Select the contact view that is furthest to the right.

Uncheck all shown contacts below the 4 pictures.

Check each contact individually to examine the different types of contacts found for the Ligand. Pay special attention to the water, hydrophobic, and hydrogen bond contacts.

**Note:** The angstrom is a unit of length equal to 10-10m ( one ten-billionth of a meter ) or 0.1 nm. Its symbol is Å. It is named after the Swedish physicist Anders Jonas Ångström (1814-1874).