DEPARTMENT OF COMPUTATIONAL BIOLOGY & BIOINFORMATICS
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Molecular Visualization Software

◇ ***Rasmol***

HANDOUT

Rasmol – an easy approach

RasMol is a visualization program created by Roger Sayle and used to display small molecules, proteins and nucleic acids. The name "RasMol" is derived from Raster (the array of pixels on a computer screen) .It is easy to use, runs on many platforms, is extremely powerful, and is free! The program can be used for analysis, display, teaching and generation of publication quality images.

1: Double click the icon named **Rasmol** in the desktop

Observation.....

2: List the name of the two window opened(You can see them on task bar at the bottom of the screen)

....

3: Write down the names of different *Menus* from the **Menu Bar** on top of the Rasmol version 2.6 Window (like File, Edit etc...)

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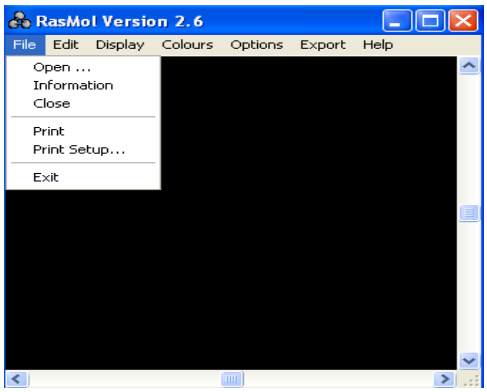
....
.....

4: Click the File Menu. Now you can see the menu options (like Open, Information etc...). Write down all the menu options corresponding to the File Menu.



…… …… ……
…… …… ……

5. Click the Edit Menu. Now write down all the menu options

…… …… ……
…… ……

6. Click the Display Menu. Now write down all the menu options

…… …… ……
…… …… ……
…… ……

7. Click the Colours Menu. Now write down all the menu options

…… …… ……
…… …… ……
…… ……

8. Click the Options Menu. Now write down all the menu options

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…… …… ……
……

9. Click the Expert Menu. Now write down all the menu options

…… …… ……
…… ……

10. Click the Help Menu, Now write down all the menu option

…… ……

11. Go to the File menu, click Open. Now a dialog box appears. (Note that for this session your files are stored in C:\Rasmol directory. For taking this from Open dialog box, double click on **My Computer -> C: -> rasmol)**

List the files available

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12. From the dialog box, select the file with name **H2O** by clicking on it and then click Open.
Observation.....

13. Now click the mouse on the screen and move it around .
Observation **.....**.....
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14 Now right click the mouse on the screen and move it around without releasing it .
Observation.....
.....

15.Now Hold the shift key and the left mouse button to zoom
Observation.....
.....

16.Now hold the shift key and press right button.
Observations.....
.....
Note: It rotates on Z axis

17: Select Display->Sticks, try to rotate by pressing the left mouse button and dragging mouse over the molecule
Observation.....

18.Select Display-> Space fill , rotate the molecule
Observation.....

19.Select Display->Ball & stick, rotate the molecule
Observation.....

20.Select Display->Wireframe, rotate the molecule
Observation.....

21.Select File->Information. Write down the details provided
Observation.....

22.Rasmol allows you to save the picture of molecule in different file formats. To save as a GIF file select Export->GIF. Now a dialog box appears. Type the file name 'Mymolecule' and save in desktop. Minimize all windows one by one. Double click the saved file. Write down your observations

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.....

23.Try for other formats in the Export menu (BMP,EPSF,PPM,RAST)
Observation.....
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24.Now we will use another molecule with a little bit more complex structure, a protein myoglobin. To open this first you have to close the already opened molecule. Select File->Close. Now you open myoglobin using File->Open.You will get myoglobin from c:\ rasmol
Observation.....

25.Try to rotate the molecule by pressing the mouse and dragging it
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26.Try all options in display menu. Write down the observation.

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27.Select Edit->Select All , even though you cannot observe anything in particular, all molecules are selected. Now we can change the colours options.

28.Select Display->ball and stick . Now Select colours->monochrome
Observation.....

29.Select colours->CPK

Observation.....

(CPK got some predefined colours for atoms Carbon: light grey ,Oxygen: red ,Nitrogen :sky blue ,Hydrogen :white ,Sulphur: yellow ,Phosphorous :orange ,Chlorine: green ,Bromine and Zinc: brown ,Calcium :dark grey ,Unknown :deep pink)

30.Select colours->Shapely
Observation.....

(Shapely: Coloured according to amino acid properties.)

31.Select colours->Group
Observation.....
(The chain is smoothly coloured from the 5' to 3' end. The colours follow the spectrum, blue, green, yellow, orange, and red)

32.Select colours->Chain
Observation.....
(The structure is coloured according to chain identity.)

33.Select colours->Temperature
Observation.....
(The structure is coloured according to temperature properties.)

34.Select colours->Structure
Observation.....
(Structure: Coloured according to secondary structure, alpha helix = purple, beta sheet = yellow, turns = blue, other = white)

35.Select Display->Ball & Stick to change display style of the molecule . Now select Options->SlabMode, A tick will appear in the menu. This mode is primarily useful for inspection of the interior portions of the molecule. Now hold down the control key, press the mouse left button and drag it from left bottom to right top . The plane will pass through the molecule. Those atoms swept by the plane will disappear from the screen. Try this and write down your observation
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.....

36.Now change the direction of mouse dragging (Hold down the control key)
What is your observation?
.....
.....

37.select Options->SlabMode, to remove the tick mark

Observation.....

38.Select Options->Labels. A tick mark will appear in the menu. Zoom through the molecule by holding shift key and dragging mouse
Observation.....

39.Select Options->Labels once again.

Observation.....

40.Select Options->Stereo.

Observation.....

41.Select Options->Stereo once again.

Observation.....

42.Select Display->Spacefill ,then select Options->Shadows.

Observation.....

43.Select Options-> Shadows once again.
Observation.....

Command Line

Command line window is opened when you open the Rasmol. It is minimized and is on the task bar. Now click on command window. You can see a Rasmol command prompt there. You can type in instruction there. Now right click on the taskbar and select Tile window vertically. You can see both window side by side. Close myoglobin and open ***Aspirin*** molecule. *When using Rasmol before opening a second file ,you have to close (File->close) the first file.* For the following questions type in commands in command line window and press Enter key and observe the Rasmol display window to see the effects. Commands are shown in bold.

44.**background white**
Observation.....

45.**select hydrogen**
colour blue
Observation.....
.....

46.**select hydrogen**
select Display->Spacefill from menu
Observation.....

47.**show information**

Observation.....
Zoom the molecule using mouse and shift key

48.**reset**
Observation.....

49.**label**
Observation.....
To see the effect Zoom in the molecule using mouse and shift key. Try to rotate.

50.**label off**
Observation.....

51.**select oxygen**
spacefill
Observation.....

52.**select oxygen**
spacefill 1.7
Observation.....

53.**Try other real values 1.3, 1.4...**
Observation.....

54.**select all**
spacefill off
Observation.....

55.**zap**
Observation.....

56.Now open Myoglobin(File->open)
Observation.....

57.**show sequence**
Observation.....

58.**set solvent true**
dots
Observation.....
Van der Waals surface is shown

59.**dots off**
Observation.....

60.**Hbonds**

Zoom into the molecule and write down the observation
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61.**Hbonds off**
Zoom into the molecule and write down the observation
.....

62.**monitor 54 60**
zoom in and out and observe the molecule
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63.**monitor off**
.....

64.**Backbone on**
Cartoon 100
Observation.....

65**. Ribbons**
Observation.....

66.**Ribbons 150**
Observation.....

67.**Ribbons off**
Observation.....

68.**Trace**
Observation.....
(produces a spline of the alpha-carbon trace)

69.**Trace off**
Observation.....

70.**Select backbone**
Colour red
Observation.....

71.**Select hydrophobic**
Spacefill
Observation.....

72.**select pro and not turn**
colour purple
spacefill 0.25
Observation.....

73.**Select 54, 100-105**
Observation.....

74.**Select ala**
Colour green
cartoon
Observation.....

75.**Select resno < 5 or resno > 40**
Colour blue
Observation.....

76.**Select within (3.0, as?)**
Observation.....
selects atoms within 3.0 Angstroms of Asp or Asn residues

77.**restrict within (3.0, as?)**
Observation.....

The restrict command will select a region and non-selected regions will no longer be shown in the representation. This is useful for examination of interior structure. To restore , select Edit->Select All, Display ->Wireframe, Colour->CPK

78.**set picking distance**
Now click on the two atoms whose distance you want to measure. Observe the command window.
Observation.....

79.**set picking monitor**
Now click on the two atoms whose distance you want to measure
Observation.....

80.**set picking angle**
Now click on the three atoms whose angle you want to measure. Observe the command window.
Observation.....

81.**set picking torsion**
Now click on the 4 atoms whose torsion you want to measure. Observe the command window.
Observation.....

Use Lysozyme for the following(Use File->Open)
82.**ssbonds on**
Observation.....

82.**ssbonds off**

Observation.....
(sulphur- sulphur bond)

Script

83.Open notepad and type in the following

Zap
Load "C:\rasmol\Lysozyme.pdb "
select all
spacefill
Echo Press any key to continue
Pause
Exit

Save as c :\ rasmol\yourscript.txt
In command prompt type in
Script yourscript.txt
Observations.....
.....
Notes:
Load filename: load a file
Exit: terminates a script but not the RasMol session
Echo: displays a message in the command line window
Pause: pauses the script until a key is pressed
Refresh: refreshes the screen

84.You may use the save script command with script option to write out a script file that will reproduce the current image.

save script myscript.

This will write a file named myscript in the RasMol directory. Now change the display style as you like. Then give the following command

script myscript
Observation.....