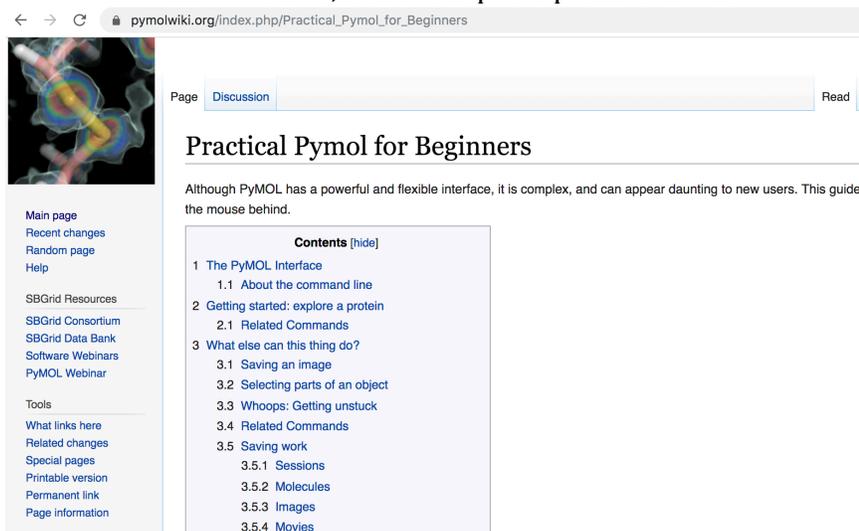


PyMol Assignment 2: Tutorial from Pymol Wiki And Creating and Manipulating Objects

Go to this webpage:

https://pymolwiki.org/index.php/Practical_Pymol_for_Beginners

Which will look like this, but the top left picture varies.



The screenshot shows a web browser window with the URL `pymolwiki.org/index.php/Practical_Pymol_for_Beginners`. The page title is "Practical Pymol for Beginners". Below the title, there is a paragraph: "Although PyMOL has a powerful and flexible interface, it is complex, and can appear daunting to new users. This guide is the mouse behind." To the right of this paragraph is a "Contents [hide]" section with the following items:

- 1 The PyMOL Interface
 - 1.1 About the command line
- 2 Getting started: explore a protein
 - 2.1 Related Commands
- 3 What else can this thing do?
 - 3.1 Saving an image
 - 3.2 Selecting parts of an object
 - 3.3 Whoops: Getting unstuck
 - 3.4 Related Commands
 - 3.5 Saving work
 - 3.5.1 Sessions
 - 3.5.2 Molecules
 - 3.5.3 Images
 - 3.5.4 Movies

On the left side of the page, there is a sidebar with navigation links: "Main page", "Recent changes", "Random page", "Help", "SBGrid Resources", "SBGrid Consortium", "SBGrid Data Bank", "Software Webinars", "PyMOL Webinar", "Tools", "What links here", "Related changes", "Special pages", "Printable version", "Permanent link", and "Page information".

Read through the page, look at the Pymol window for every button and feature mentioned, perform the actions as directed in this tutorial, including loading the PDB file 1BL8, which is potassium channel protein from *Streptomyces Lividans*, and saving an image that looks like that shown for this protein shown in the tutorial.

Going beyond the tutorial, enter the following in the command line:

PyMOL>reinitialize (resets Pymol to its initial state)

PyMOL>fetch 1AHO (to load in the structure of the scorpion protein toxin).

PyMOL>bk_ground white

Look on the RH side of the Pymol window and you will see

all ASHL C

1AHO 1/1 ASHL C



"1AHO" is the object that contains the coordinates of the protein you have downloaded. ASHLC are pull-down windows.

A = actions

S = show

H = hide

L = label

C = color

On the 1AHO panel

Click H

Click Everything (hides everything; everything should disappear)

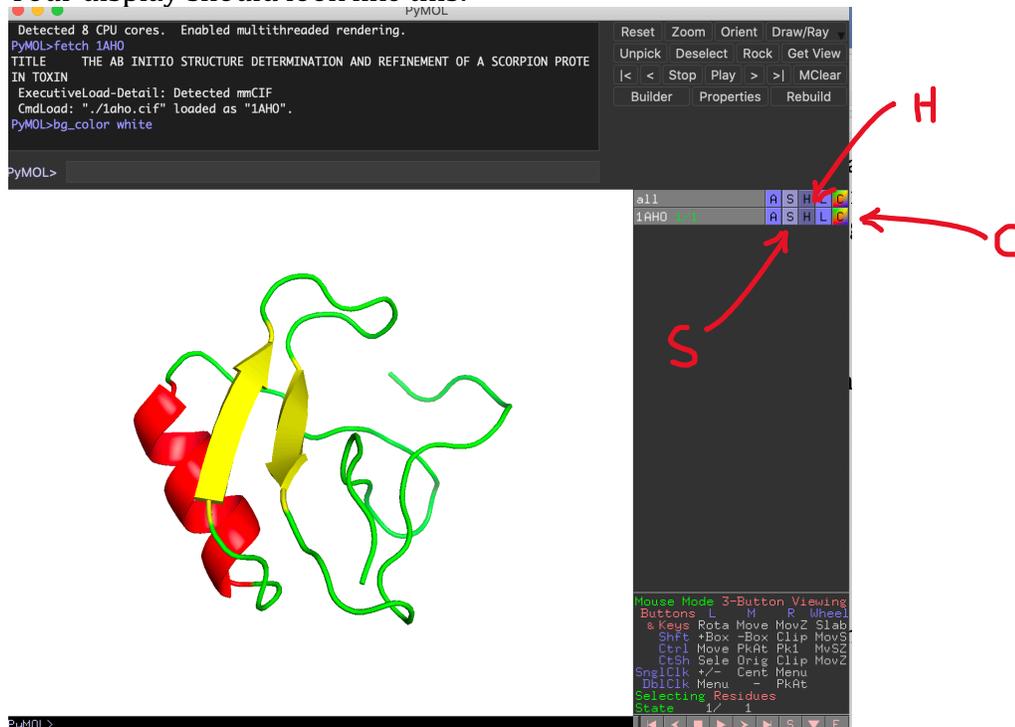
Click S

Click Cartoon (show cartoon; the protein will show as a cartoon)

Click C

Click by ss (color by secondary structure; the loops, helices and β -strands show in different colors)

Your display should look like this:



PyMol allows you to make as many “objects” as you like, each with its own set of attributes. To illustrate this feature, and how to work with objects, make objects from subsections of this protein that are associated with different elements of secondary structure.

type

PyMOL> create loop1, resi 1-18

all	A	S	H	L	C
1AHO 1/1	A	S	H	L	C
loop1 1/1	A	S	H	L	C

Now you have three objects.

all is there by default and you will not use it.

1AHO contain the protein plus all the waters, ions and ligands in the 1AHO coordinate file.

loop1 contains residues 1-18 of the protein.

Now go to “H” button of loop1 and hide everything, then show it as stick

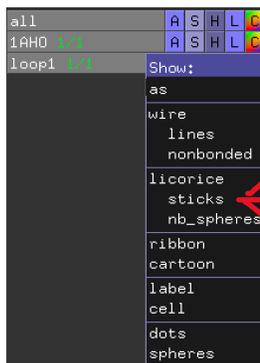
Click H (of loop 1)

Click everything

Click S (of loop 1)

Click S

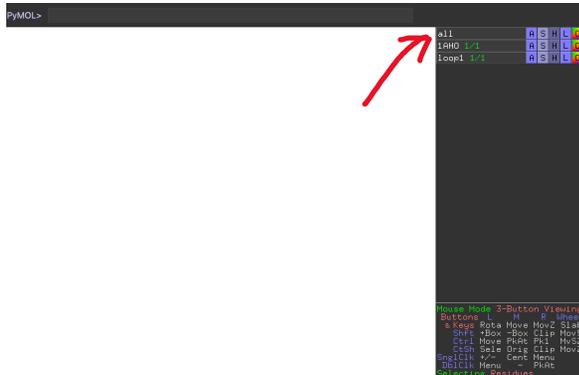
Click licorice sticks



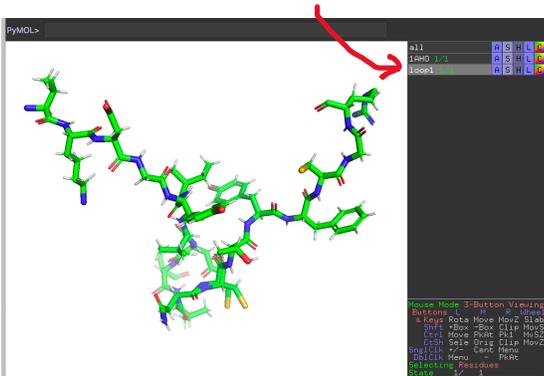
Click C

Click by element (color atoms by element type)

Turn all objects off by clicking on all



Turn on loop1 by clicking on loop1



Now make more objects. Make objects for the all the structural elements of this protein. Type
PyMOL> create helix1, resi 19-28
PyMOL> create loop2, resi 29-32
PyMOL> create sheet1, (resi 33-37 or resi 44-49)
PyMOL> create loop3, resi 38-44
PyMOL> create, loop4, resid 50-64

The sidebar should look like this

all	A	S	H	L	C
1AHO 1/1	A	S	H	L	C
loop1 1/1	A	S	H	L	C
helix1 1/1	A	S	H	L	C
loop2 1/1	A	S	H	L	C
sheet1 1/1	A	S	H	L	C
loop3 1/1	A	S	H	L	C
(sele)	A	S	H	L	C

When you get to this point be sure to use the Save State As... feature to save your work, so that you can come back to it later, if you need to, or so that you can go back to a particular point if you make an error.

Turn off 1AHO

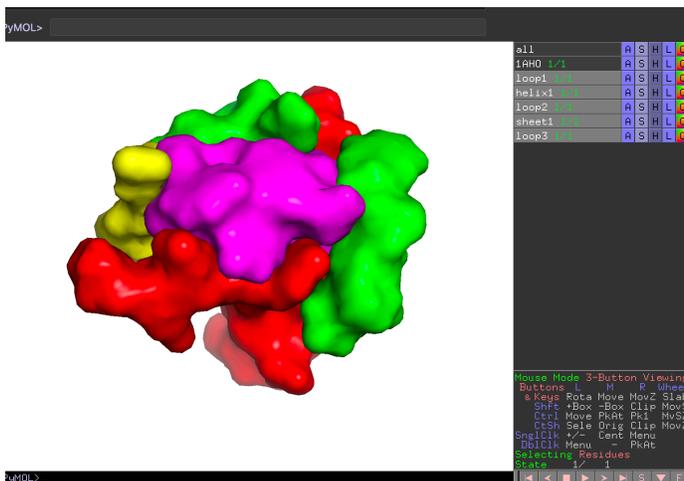
Turn on all the objects you have made.

Make each of your object into a surface representation (H everything, S, surface)



Give each object a different color

It should look something like this.



Send a ray 2000,2000 image to Loren