Pymol Assignment 3: The Progesterone Receptor Protein

In this assignment you will practice selecting parts of molecules using different identifiers, including chain, residue name, and residue number. You can find more terms for selecting parts of molecules at the PyMOLWiki:
https://pymolwiki.org/index.php/Property_Selectors

Start by copying and pasting the entire text here between start and end, all at once, into the Pymol command line. Then press carriage return.

```
----------start----------
# delete all objects and reset pymol
reinitialize
# set the background color to white
bg_color white
# make the background transparent for ray trace
set ray_opaque_background, 0
# set the ray trace mode
# normal color
set ray_trace_mode, 0
# normal color + black outline
#set ray_trace_mode,  1
# black outline only
#set ray_trace_mode,  2
# turn off shadows during ray trace
set ray_shadows, 0
# set the mouse mode for laptop.
config_mouse one_button
# get rid of double bonds and skinny bonds to H
set stick_h_scale, 1
set valence, 0
# high quality surfaces
set surface_quality, 3
----------end----------
```

Now load the protein

PyMOL>fetch 1A28

It seems fetch does not work from China, so alternatively go the PDB website, and download 1A28.pdb to your computer.

Then load it directly into Pymol
PyMOL>load 1A28.pdb

[or possibly PyMOL>load Downloads/1A28.pdb, depending on where your computer put the file]

Part I Cleaning up
This protein is functional as a monomer, but crystallizes with two protein molecules in the asymmetric unit. This happens quite often, so you will see multiple copies of a protein in Pymol. Generally we need to remove all but one of these copies. Some water molecules are also observed that we won't need (remember that crystallographers have a hard time seeing hydrogen atoms so water molecules lack hydrogens). We will focus on just one copy of the protein and will omit the waters.

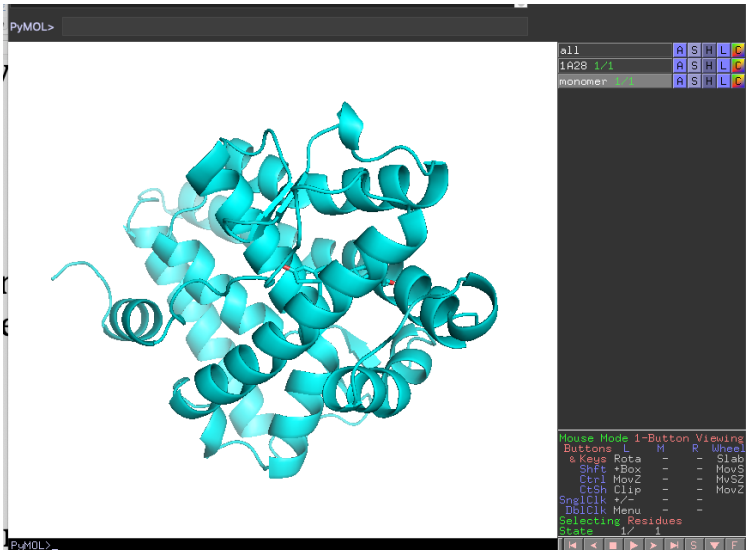
Once you load or fetch, the protein dimer of 1A28 and its waters are an object within Pymol, shown on the RH side. We can make a new object in Pymol that is only Chain A (one of the two protein molecues) of the dimer and with no water molecules.

PyMOL> create monomer, chain A and not resname HOH

Now turn off object 1A28 on the RH panel (make it invisible) by clicking on its button. You should now only see your new object (monomer), which contains a single polypeptide chain of the original protein without any waters.

Center it
PyMOL> center monomer

This command places the rotational center at the center of the protein monomer. You should see this.



monomer is now centered in the window, and when you spin the protein using the mouse or track pad it rotates about the center of mass of Chain A.

Now remove the original protein object (this cannot be undone).

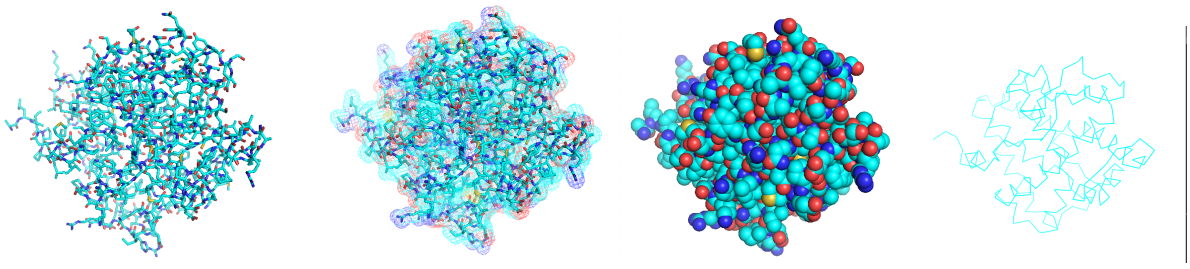
PyMOL> delete 1A28

Part II Representations

Experiment with various representations of the monomer. Using the S (show) and H (hide) buttons on the RH side. Show the protein as sticks, sticks + mesh, ribbon, cartoon, dots, spheres, mesh and surface.

For example.

stick stick+mesh sphere ribbon



Ray trace each of your images, and save them as pngs. Put them all on one page in a word doc.

Part III Hydrophobic Amino Acids

Represent your protein as a cartoon, and make it red.

PyMOL>color red, monomer

Make the hydrophobic amino acids blue

PyMOL> select hydrophobes, (resn ala+gly+val+ile+leu+phe+met+trp+tyr) and monomer
PyMOL>color blue, hydrophobes

What do you notice about the general distribution of hydrophobic amino acids?

PyMOL> create one_helix, (resid 838-858) and monomer
PyMOL>center one_helix
H (hide) everything for one_helix
S (show) sticks for one_helix.

Make an image viewing directly down the helical axis and several images viewing perpendicular to the helical axis. What do you learn about alpha helices from this? Add the images to the word file for this exercise and email it to your professor