Pymol Exercise
CHEM 6572
Scripting and working with directories
        In this exercise we will explore methods for navigating, programing and automating Pymol.

A) Download the PDB entry for structure 1A4Q. (i.e., get the file called 1A4Q.pdb from the PDB).
This is the influenza virus neuraminidase complexed with 2-dihydropyran-phenethyl-propyl-carboxamide.

Create a directory called neuraminidase on your desktop and put 1A4Q.pdb into this directory.
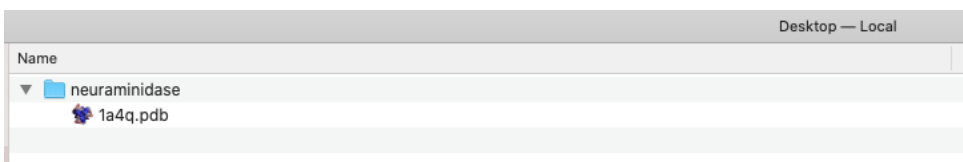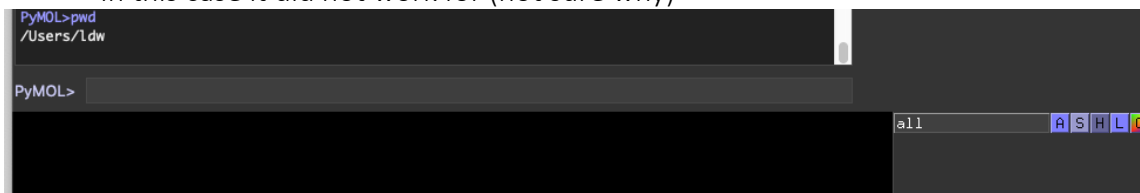

B) Launch Pymol without loading a coordinate file
        (alternatively launch Pymol by double clicking on a pdb file, then type "reinitialize")

        Set the working directory to your neuraminidase directory
File → working directory → File Browser
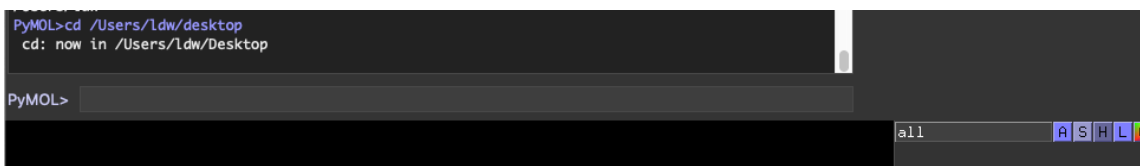   Use pwd to ensure this works
        In this case it did not work for (not sure why)

Use cd to set the directory
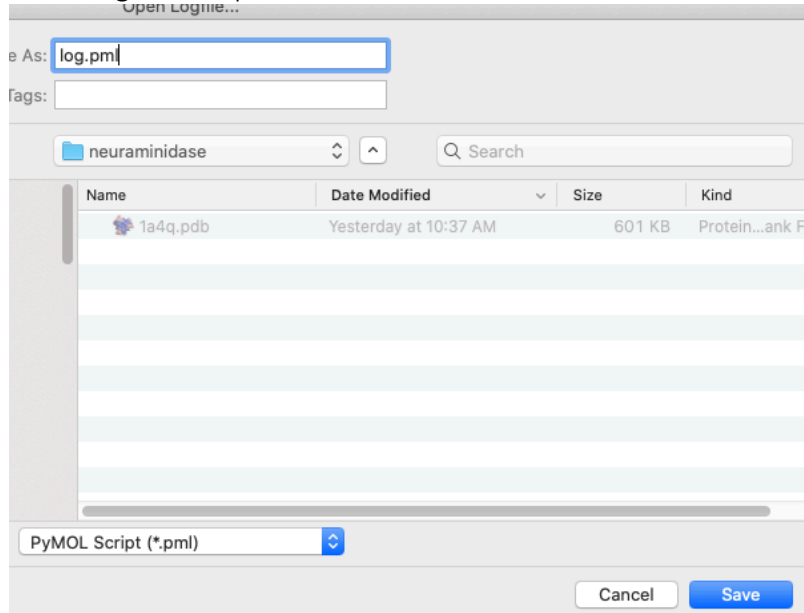cd /Users/ldw/desktop
(note that the directory of each computer is different and you will have to adapt the directory command to your computer).

C) Start Logging

Start loggin your commands, and save the log file to the neuraminidase folder under then name log.pml.

File→Log File→Open

Set up Pymol as previously by copying and pasting the following into the command line [note that the reinitialize command is commented out. If you reinitialize you will turn off logging]

```
#----------------------------------------------------------------------------
## Header: General Commands ##

# 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 of Header: General Commands
#---------------------------------------

D) Load the 1A4Q.pdb into Pymol
        load 1A4Q.pdb

Remove extra copies of the protein and water molecules
        create protein, chain A and not resn HOH
        delete 1A4Q

make the protein blue
        color blue, protein

make the protein cyan
        color cyan, protein

make the calcium ion orange
        color orange, resn CA

color the atoms of the 2-dihydropyran-phenethyl-propyl-carboxamide.
        color wheat, name C* and resn DPC
        color red, name O* and resn DPC
        color blue, name N* and resn DPC

Click randomly on three or four atoms to see their names above the command line.

Go to File→Log File→Close

E) Run your log file as a script

Set Pymol back to the initial state
        reinitialize

Run the log file
        @log.pml
This should bring Pymol right back to the state where you closed the log file.

F) Edit your script.
Go to your neuraminidase folder (with your OS, not in Pymol) and copy log.pml to neuraminidase.pml.

In the Pymol command line, type
        ls
"ls" lists the contents of the neuraminidase folder to show you the neuraminidase.pml file

Open neuraminidase.pml in a text editor or in Word (if you use word you have to save as 'text only').

Look at the script file and you should see the commands you used in your Pymol session.

The first part of the file should look like this
        load 1A4Q.pdb
        #---
        ## Header: General Commands ##
        # 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 of Header: General Commands ##

It is important, if you are going to run a script over and over and edit it each time (you are going to do this), that you reinitialize each time. If you reinitialize you will ultimately crash Pymol. Therefore, uncomment the reinitialize statement

        Change
                #reinitialize
        to
                reinitialize

But if you reinitialize after you load the pdb file, you will simply undo the load.
Move the load statement to the end of the General Commands (after the reinitialize command).

        #---
        ## Header: General Commands ##
        .
        .
        .
        set valence, 0
        # high quality surfaces
        set surface_quality, 3
        ## End of Header: General Commands ##
        load 1A4Q.pdb

Once you have moved the load statement, save the file (you don't have to close it)

Run the file in Pymol

        @neuraminidase.pml

This should not do anything, because you are starting and ending in the same state.

In your editor, find and delete all the commands related to clicking on atoms. They don't do anything but clutter your script.

In my file those commands look like this.

cmd.select('sele','none')
cmd.select('sele',"byresi((((sele) or byresi((protein`15))) and not ((byresi((protein`15))) and byresi(sele))))",enable=1)
color orange, resn CA
cmd.select('sele',"byresi((((sele) or byresi((protein`3076))) and not ((byresi((protein`3076))) and byresi(sele))))",enable=1)

```
        color wheat, name C and resn DPC
cmd.disable('sele')
cmd.select('sele','none')
cmd.select('sele',"byresi((((sele) or byresi((protein`3076))) and not
((byresi((protein`3076))) and byresi(sele))))",enable=1)
```

Also delete the viewport commands
```
        _ viewport (\
        _   752.000000000,  970.000000000 )
```

The remaining commands, after the header, should look like this.

```
        load  1A4Q.pdb
        create protein, chain A and not resn HOH
        delete 1A4Q
        color blue, protein
        color cyan, protein
        color wheat, name C* and resn DPC
        color wheat, name C* and resn DPC
        color red, name O* and resn DPC
        color blue, name N* and resn DPC
```

Delete the first color command (color blue, protein), since it is overruled by the second color command.

Edit your script
        Change
                color cyan, protein
        to
                color red, protein

Save your script, but do not close it.
Run it in Pymol

        @neuraminidase.pml.

The protein should turn red

Edit your script again by pasting the following to the end of the file.
```
        set_view (\
        0.982923865,      0.174702242,     -0.057773039,\
        0.140517563,     -0.509949803,      0.848649442,\
        0.118799858,     -0.842277408,     -0.525790095,\
       -0.000009970,     -0.000051025,    -61.349761963,\
```
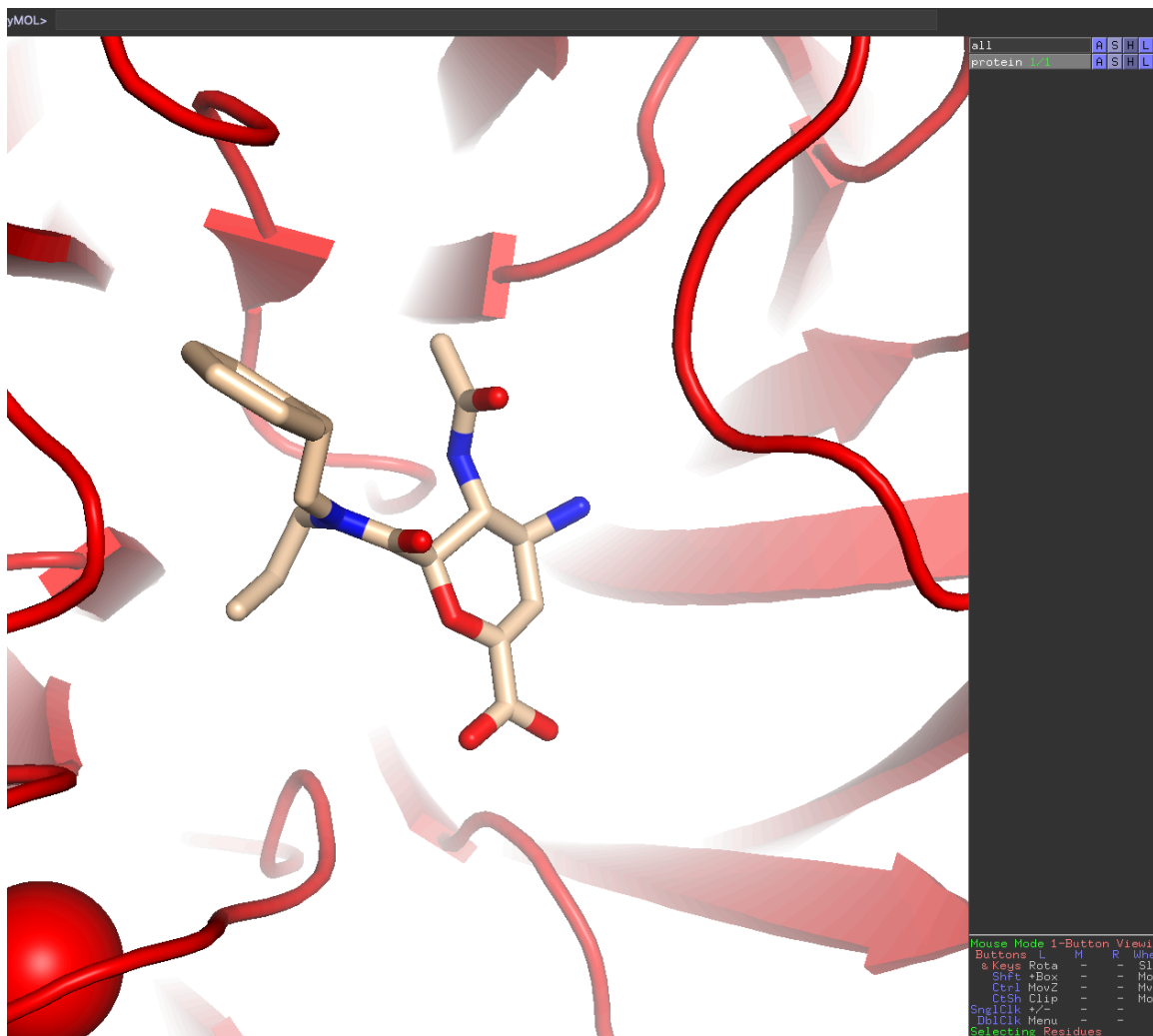
```
    -2.409132957,    57.839839935,    -9.423425674,\
    45.392078400,    77.302650452,   -20.000000000 )
```

Run Pymol

       @neuraminidase.pml.
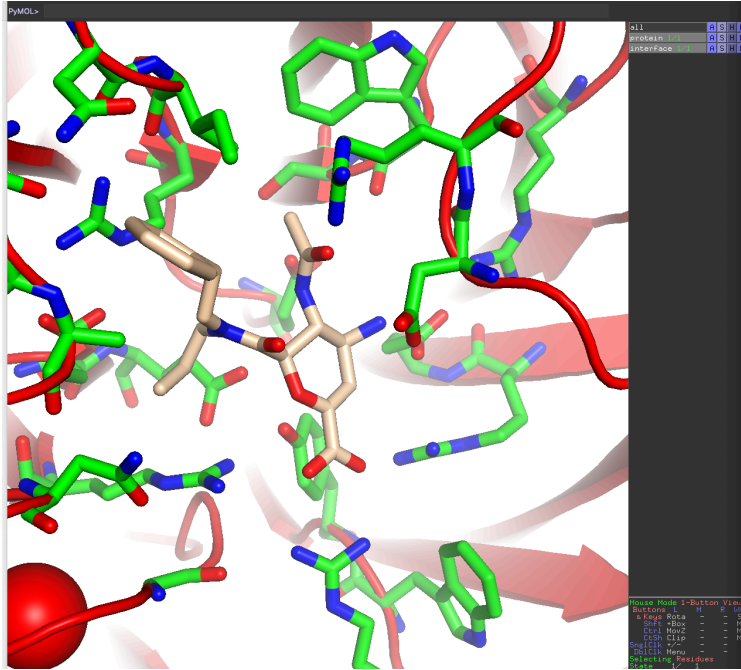
you should see this

Insert the following commands before the set_view command

create interface, byres((protein and not resn DPC) within 5 of resn DPC)
side everything, interface
show stick, interface

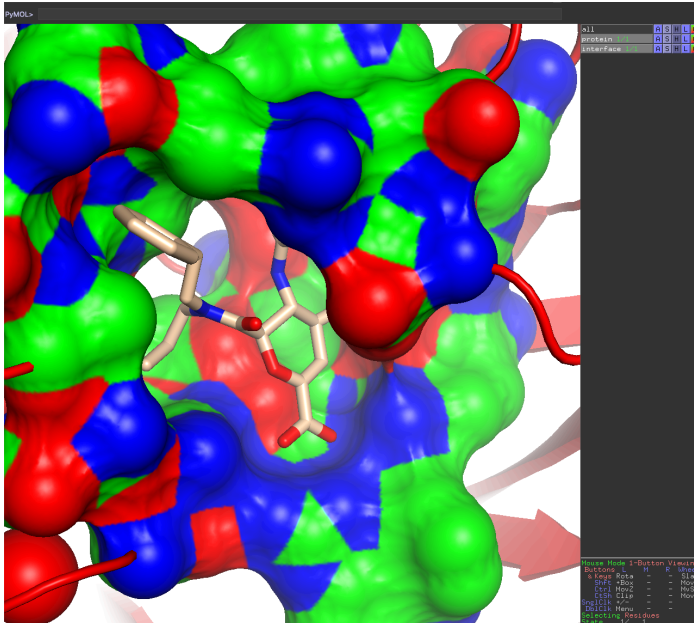Run Pymol

@neuraminidase.pml.

you should see this

Insert the following command before the set_view command

show surface, interface

Run Pymol

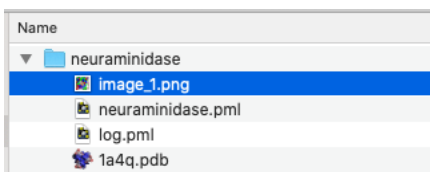@neuraminidase.pml.

you should see this

Insert the following command **after** the set_view command

        ray 1000,1000
        save image_1.png

Run Pymol

        @neuraminidase.pml.

you should see this in your directory

At the end of the file insert the following commands

        h_add resn dpc
        ray 1000,1000
        save image_2.png

Run Pymol

        @neuraminidase.pml.

You should see this in the Pymol window:

you should see this in your directory

In the end your script should look like this

```
# 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 of Header: General Commands ##
load  1A4Q.pdb
create protein, chain A and not resn HOH
delete 1A4Q
color red, protein
color wheat, name C* and resn DPC
color red, name O* and resn DPC
color blue, name N* and resn DPC

create interface, byres((protein and not resn DPC) within 5 of resn DPC)
hide everything, interface
show stick, interface


color green, name C* and interface
color red, name O* and interface
color blue, name N* and interface

show surface, interface

set_view (\
 0.982923865,   0.174702242,  -0.057773039,\
 0.140517563,  -0.509949803,   0.848649442,\
 0.118799858,  -0.842277408,  -0.525790095,\
-0.000009970,  -0.000051025, -61.349761963,\
-2.409132957,  57.839839935,  -9.423425674,\
45.392078400,  77.302650452, -20.000000000 )

ray 1000,1000
save image_1.png

h_add resn dpc
ray 1000,1000
save image_2.png
```