Assignment 1 kickstart

1. Accessing PyMol:

- Option 1 (recommended): Use the in-person LTS machines, which have PyMOL already downloaded
- Option 2: log in remotely to an LTS machine according to this handout
- Option 3: Download PyMOL from the Robin Li and Melissa Ma Science Library website. The University has a campus-wide license agreement for PyMOL, and can be accessed here (simply scroll down to the Academic and Non-Profit Price List, and click to determine if your institution has a site-wide PyMOL Subscriber. If you are on Stanford wifi, or using a Stanford VPN, you should receive a license file download.)

2. **Visualizing Proteins**
    a. Refer to PyMOL tutorial
3. **Secondary Structure Elements**
    a. Refer to PyMOL tutorial

4. Ramachandran Plots, and Coding in PyMOL

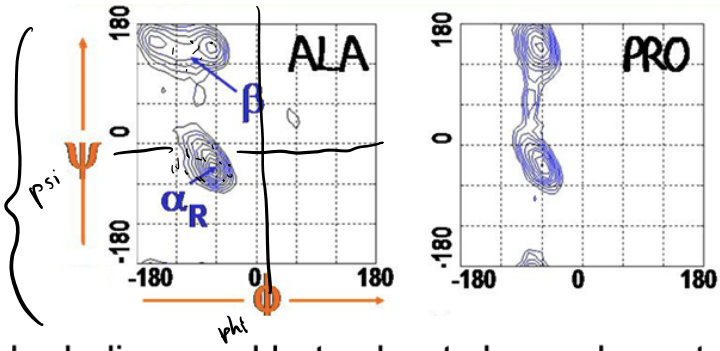
```
def ramachandran(sel):
    """
    Produce a Ramachandran plot for residues in the given selection.
    """
    cmd.delete('phi')
    cmd.delete('psi')
    resnums = get_residue_numbers(sel)
    phis, psis = [], []
```

```
# For each residue in resnums, add the phi and psi angle to phis and psis, respectively.

# PyMol has two commands related to dihedral angles:
# cmd.dihedral(name, sel1, sel2, sel3, sel4) will plot the dihedral on the
#     structure however it will not return the value.
# cmd.get_dihedral(sel1, sel2, sel3, sel4) will return the dihedral but will
#     not show it on the structure.

# Only cmd.get_dihedral is strictly required in your implementation, but
# we highly recommend that you call both commands with the same selections
# so that you can visually see the angles for debugging purposes.
# Note that cmd.dihedral has an additional ``name'' argument, which you
# should set to "phi" for the phi angles and psi for the "psi" angles.

# Some tips on what various error messages mean:
# "Error: Selection 1: Not found": The first selection matches no atoms.
# "Error: Selection 1: Invalid selection name": The first selection matches multiple atoms.
# Equivalent messages for Selection 2 mean the second selection is invalid, and so on.

################################################################################
# Edit here.

################################################################################
plt.scatter(phis, psis)
plt.xlabel('phi')
plt.ylabel('psi')
plt.ylim(-180, 180)
plt.xlim(-180, 180)
plt.gca().set_aspect('equal')
plt.show()
```

From “Biomolecular Structure” lecture:

Ramachandran diagrams

- A plot showing a distribution in the (Φ, Ψ) plane is called a Ramachandran diagram
  - Such a diagram can be a scatterplot, or a two-dimensional histogram visualized as a contour map or heat map
  - For example, one might make a Ramachandran diagram for many residues of the same amino acid type
- Some amino acid types have distinctive Ramachandran diagrams

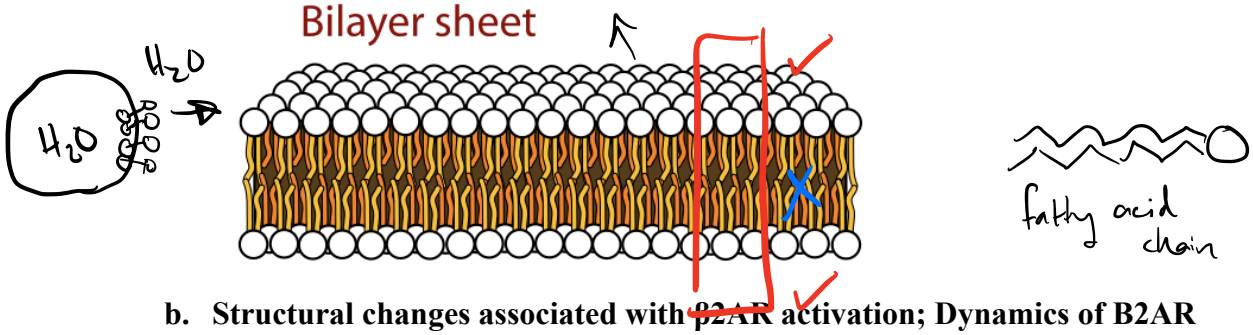


Ala is typical
Pro is unusual

Image from
Michael Levitt

- Alpha helices and beta sheets have characteristic Ramachandran diagrams

5. **Visualizing Nucleic Acids**
   a. Refer to PyMOL tutorial
6. **Structure and dynamics of the β2 adrenergic receptor**
   a. **B2AR's home in the cell membrane**
      i. How can you find what types of molecules are present in the system?
      ii. Review phospholipid bilayer:



   b. **Structural changes associated with ~~β2AR~~ activation; Dynamics of B2AR**
      i. What are some conditions that might need to change in order to allow the nanobody to bind?

ii. Explore the structures visually — good practice is to name your selections so you can come back to them. >> name sele, <name>

c. Analysis of RMSDs

i.