(I) Download the structure of the Catalase enzyme (1JKU) from the PDB Databank. Open the structure in Jmol and use the command "rama" or 'ramachandran". Compare the result to the same plot for the Ribonuclease (entry 1DY5 in the protein data bank) and the silk protein Fibril (3UA0). Give a short answer to the following questions:

1. What is presented on the plot created by Jmol?
2. What is the meaning of the different colors on the plot? Do the positions of the differently colored amino acids on the Ramachandran plot match the theoretical predictions?
3. Describe the differences between the secondary structures of the three proteins.

(II) Use Jmol to calculate the potential surface for different Ψ and Φ angles of the middle aminoacid in a tripeptide.
Several tripeptides are uploaded on the server (https://kvv.imp.fu-berlin.de/portal → Biophysik für Bachelor → Resources → Übung 2)

1. Open the Gly-Ala-Gly polypeptide in Jmol. Measure the Ψ and Φ angles. Part of which type secondary structure can this polypeptide be? Do you know a protein where there is such an alteration of these two amino acids?
2. Use Jmol to calculate the potential energy for the Gly-Ala-Gly polypeptide. Jmol command:
   $ minimize energy
3. Calculate a 2-dimentional potential curve for three different Ψ angles varying the Φ angle in the range from -180° to +180° (step of 10°). Present graphically these potential curves as a function of Φ (use another program for making the plot, e.g. Origin, Excel, Mathematica or Matlab).
4. Calculate the 2-dimentional potential curve for three different Φ angles varying the Ψ angle in the range from -180° to +180° (step of 10°). Present the results in a graphic form.
5. As an alternative to tasks 3 and 4 you may calculate one 3-dimentional plot varying both angles with a step of 10°. Use the script provided on the server. Use Jmol command:
   $ script pot_GlyAlaGly.txt
   Present the results graphically (as a 3D plot).
6. Compare the two force fields used in Jmol (MMFF94 and UFF force fields). Repeat tasks 3 and 4 (or task 5) using different force field. To change the force filed used by Jmol type:
   $ set forcefield "UFF"
   or
   $ set forcefield "MMFF"
7. Using one of the force fields make a potential energy plot (2D or 3D) for one of the other tripeptides uploaded on the server. Compare the potential energy plot to this for the GlyAlaGly tripeptide. Discuss the differences.