**Structural Bioinformatics (Biochemistry and Biophysics 670, Bioinformatics and Computational Biology 717)**

**Lectures:**

**Recitation:**

**Instructor:** Konstantin Popov, GMB 3044, [kpopov@ad.unc.edu](mailto:kpopov@ad.unc.edu), office hours by appointment

**TAs:**

**Course prerequisites:** Enrolled as a graduate student in the biological sciences. To complete your assignments, you will need to do some scripting in Python. Also, minimal scripting in bash shell enjoinment will be required.

**Course goals:** Outline general problems ofcomputational structural biology and computational drug discovery. Explain common approaches and corresponding computational tools for protein structure prediction, design, and analysis. Students will learn how to perform this analysis using various computational platforms available for scientific community.

**Dates:** Each week a homework involving modeling with various computational tools will be assigned.

Grades will be determined (Fail, Low Pass, Pass, High Pass) based on the assigned programming exercises and class participation.

**Lecture Schedule:**

Lecture 1: Introduction to proteins

Lecture 2: Protein structure, stability and folding

Lecture 3: Computational tools for protein structure visualization and manipulation

Lecture 4: Molecular dynamics (MD) for protein folding and structure prediction

Lecture 5: Multiple sequence alignment and homology modeling

Lecture 6: Introduction to Machine Learning for structural biology

Lecture 7: Machine learning for protein structure prediction and design

Lecture 8: Protein-ligand interactions, computer assisted drug discovery

Lecture 9: Open questions in computational structural biology

**Assignments:**

1. BioPython homework
2. PyMOL homework
3. Gromacs MD simulation homework
4. AlphaFold homework 1
5. AlphaFold homework 2
6. Identification of potential druggable sites on the protein surface