BioSci 2147, Protein Structure and Function fall 2013
Instructor: Dr. Grabe

Lecture	Date	Topic	Content/Reading
1	08/27	Introduction	
2	09/03	Molecular forces I	Electrostatics, ion screening, intermolecular interactions
Molecular Driving Forces by Dill: Chapters 20, 21, 22, 23 Ion stability paper by Roux and MacKinnon (1998) Science **285**:100			
3	09/10	Molecular forces II	intermolecular interactions, properties of water
Molecular Driving Forces by Dill: Chapters 24, 29, 30, Gecko van der Waals papers by Autumn et al. (2000) Nature **405**:681, Autumn et al. (2002) PNAS **99**:12252			
4†	09/17	Unix/programming	Introduction to the Unix shell and text editor
Overview of Unix terminal and text editors: Git-Bash (http://msysgit.github.io/) - shell for Windows users Sublime Text (http://www.sublimetext.com/) Zed Shaw's "Command Line Crash Course" (http://cli.learncodethehardway.org/book/)			
5	09/24	Protein structure	Protein building blocks, folds, experimental techniques: X-ray, NMR, EM
Molecular Driving Forces by Dill: Chapters 1, 5, 6 Proteins by Creighton: Chapter 6 X-ray structure paper by Wiener et al. (2012) Nature **483**:618			
6	10/01	Functional methods/Quiz	FRET, DEER, cystein scans, chemical crosslinking, biotin avidin, Quiz #1
Proteins by Creighton: Chapters 5.2, 5.4, 7.5.4 DEER study by Claxton et al. (2010) Nature Structural & Molecular Biology **17**:822 MTSET scanning paper by Larrson et al. (1996) Neuron **16**:387			
7	10/08	Kinetics	Chemical kinetics, experimental methods, single molecule
Molecular Driving Forces by Dill: Chapter 19, 28 SmFret paper by Ferreon et al. (2012) Nature **498**:390 Thrombin/antithrombin paper by Olson and Shore (1992) JBC **257**:14891			
--	10/15	No class	
8	10/22	Homology models	Sequence alignment, blast, homology modeling
Handouts written by Dr. Grabe will be provided VDAC X-ray paper by Ujwal et al. (2008) PNAS **105**:17742			
9	10/29	Protein design	Classic studies in engineering protein folds
Design of 4-helix bundle by Ho and DeGrado (1987) JACS **109**:6751 Design of globular protein by Kuhlman et al. (2003) Nature **302**:1364 Design of a β-sheet by Kortemme et al. (1998) Science **281**:253			

10	11/05	Molecular simulation I	Theory of molecular simulation – Newton's laws, classical force fields, numeric approaches
Understanding Molecular Simulation by Frenkel and Smit: Chapter 4 Classic MD simulation paper by McCammon et al. (1977) Nature **267**:585 Overview of current simulation methodologies Dror et al. (2012) Annual Review of Biophysics **41**:429			
11†	11/12	Molecular simulation II	Molecular dynamics tutorial – simulation of water movement through gramicidin A
Tutorial on MD simulation setup, run, and analysis written by Dr. Joshua Adelman: http://synapticarbors.github.io/BioSci1540/			
12	11/19	Molecular simulation III	Practical molecular simulation – analyze simulation results
Use VMD to watch and analyze simulations from lecture 11			
13	11/26	Protein/ligand docking	Protein-protein docking and drug discovery/drug docking
Review of ligand/drug docking by Huang et al. (2006) Physical Chemistry Chemical Physics **8**:5166 Classic protein-protein docking study by Katchalski et al. (1992) PNAS **89**:2195			
14†	12/03	Quiz/In class work	Quiz #2 and in class work on final projects
Final quiz and free time to work on final projects			

† - I will be traveling on these days so class will be led by Dr. Adelman and/or Dr. Pendse from the Grabe lab.

Texts used:
Molecular Driving Forces: Statistical Thermodynamics in Chemistry & Biology by Ken A. Dill and Sarina Bromberg
Proteins: Structures and Molecular Properties by Thomas E. Creighton