Advanced Protein Biophysics PHOL 475 (Bioc/Chem/Pharm/Sybb) Spring Term'13 Tues/Thurs 4.00-5.30pm Rm. E614:

Part A: Protein Structure:
from basic theory, to conceptual applications and their realization

Jan.		
15	MB/LZ	1: ***Organizational*** : Introduction to course & NAMD/CHARMM
17	MB	2: Structural Modeling and conformational search/minimization
22	MB	3: Modeling Protein Dynamics
24	MB	***4: Computational hands on: Minimization and Dynamics***
29	MB	5: Conformational Change and Energy Coupling
31	SY	6: Electrostatics
Feb.		
2	SY	***7: computational hands on: Electrostatics/Poisson Boltzmann***
4	TR	8: Equilibria, Binding and Cooperativity
7	TR	9: Equilibria, Binding and Cooperativity cont.
12	TR	10: Probability and Entropy, Statistical Mechanics
14	WS	11: Temperature & Heat Capacity, Water, the Hydrophobic effect
19	WS	12: Equilibrium Folding; H/P model & Helix Coil-Theory;
21	WS	13: Protein Folding Kinetics, Intermediates & Misfolding
26	WS	14: Amyloid Diseases
28	MB/LZ	***15: computational troubleshoot with trajectory analysis***
Mar		
5	no class	
7	MB/TR/WS	***16: Student presentations***
12		**17: mid-term exam**

Part B: Protein Conformations, Dynamics and Function

14	SC	18: Protein-lipid interactions
19	SC	19: Membrane Proteins
21	SC/LZ	20: Membrane protein modeling and simulations
26	RR	21: Diffusion and Transport
28	RR	22: Molecular Machines
Apr.		
2	RR	23: Protein Dynamics in Modern Enzymology
4	RR	24: ***computational hands on: protein machines***
9	SB	25: Intrinsically unstructured proteins
11	no class or guest lecture	
16	*no class*	
18	*SC/RR*	***26*****: Student Presentations**
23		**27: end-term Exam**

Participating Faculty: Matthias Buck (Course Director); Sudha Chakrapani; Tomasz Religa; Rajesh Ramachandran; Witold Surewicz; Sichun Yang (Proteomics and Bioinformatics); Liqun Zhang, Susmita Borthakur

Text-books: A. Fersht Structure & Mechanism in Protein Science
J. Goodrich & J. Kugel, Binding and Kinetics for Molecular Biologists
T. Creighton Proteins: Structures and Molecular Properties
M. Luckey Membrane Structural Biology

Course Description: Structural, thermodynamic and kinetic aspects of proteins will be considered in the context of fundamental biophysical theories and concepts used to describe them. The application of these theoretical frameworks will be illustrated with examples from the literature by papers selected for student presentation.

The course will be interleaved in a 1/2 discussion/seminar, 1/4 practical computational work and 1/4 student presentation format. Students will find considerable variation by instructor. However, unless told by the instructor otherwise, they should study the materials given for each session by the individual instructors BEFORE the class and engage with the questions posed. Paper/text-book material discussion may form part of the seminars and class participation will be evaluated at 1/4 of the total grade. If in doubt students should ask the instructor, before the class.

Student presentations will be on one of the topics given by the instructor. Two students will present at each session. In order to facilitate discussion each presentation/ paper will also be assigned to one other student, who is not presenting. Student presentations and hands on computational work will account for 1/4 of the total grade.

If a Student misses a class for a valid reason, such as illness, personal/family emergencies, this is to be given to instructor and the course director by noon of the day of the class. The student will then be asked to compose a written critique – a 2 page report – on a research paper or text material chosen by the instructor. The report must be submitted within 1 week of the excused absence.

Computational hands-on exercises: The molecular mechanics/dynamics program NAMD/CHARMM will be used for all these exercises. Program scripts and instruction will be provided to run the simulation and some of the analysis. The scripts may need to be slightly altered to extend the analysis and it is up to the student to plot molecular structures and parameters using VMD in conjunction with their favorite graphics software. It is expected that all simulations can be started in-class and problems mostly be resolved there. A 2-3 page report, incl. Figures, should be turned in for grading before the next class. The report consists of the results of the simulation/analysis and answers to specific questions.

The mid- and end-term exam will comprise 1/4 of the total grade each. The exams will consist of 6-7 essay type questions corresponding to the classes lead by the instructors (i.e. excluding the student presentation sessions). Students will have 60mins to answer 4 questions of their choice.