

Biochemistry & Molecular Biology 961 (BMB961)

aka CMSE 890 section 1

Concepts in Biomolecular Structure and Modeling

Spring 2017

Lecture: Tuesdays 3-4pm in room 183 Chemistry

Lab: 2 hours, on Thursdays 2-4 in 202 Biochemistry

Credits: 2

Prerequisites: Biochemistry 803 or detailed knowledge of protein and nucleic acid sequences and structures are highly desirable; previous experience with computers useful but not required; enrollment only by permission of the instructors.

Enrollment limit: 15

Instructors:

Dr. Michael Feig (432-7439; 218B BCH),

Dr. Alex Dickson (884-8985; 316C BCH),

Dr. Kaillathe (Pappan) Padmanabhan (course coordinator; 353-0814; 202A BCH),

Course description:

This is a hands-on course revolving around computational methods for the modeling of biomolecular structure and dynamics. We will begin with a brief introduction into UNIX basics, molecular graphics visualization software, and basic tools for data analysis and plotting. We will then cover protein structure prediction from sequence, homology modeling and describe different levels of computational models for biomolecules and techniques for docking and binding free energy estimates. To study the dynamics of biomolecules we introduce molecular dynamics simulations, enhanced sampling methods, clustering and kinetic network models as well as normal mode analysis. Finally, we will cover specific challenges in setting up and analyzing simulations of membrane and nucleic acid systems and finish with a perspective for how to relate simulation data to experiments. Lectures will cover the theory and demonstrate the computer methods used; lab hours will provide hands-on experience. During the last two weeks, students will develop and present research proposals to carry out computational studies that could complement experiments.

For more information and permission to enroll, please contact Kaillathe (Pappan) Padmanabhan (padmanab@msu.edu). Please also submit an override request at <http://www.bmb.msu.edu/undergraduate/override-request/>.