INTRODUCTION TO
COMPUTATIONAL BIOLOGY

BS M123, CS 183, MB 223

Humanities Hall - HH 143 (#601)
TuTh 11:00am -12:15pm

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Syllabus

This is an introduction to structural molecular biology using computational methods. Besides providing a fundamental background in biochemistry and molecular biology, it also surveys a wide variety of applications to the current biomedical research fields. Its aim is to give an introduction of the biological problems that arise and how computational methods are developed to address them. It does not train students to be expert users of specific methods, but train students to appreciate the basic ideas of the methods and how the methods are used in the analysis of biomedical questions.

Student involvement in the classroom is an integral component for this course. Successful completion of the course will benefit students in the following crucial areas that are often overlooked in other classes on campus: (a) developing skills to summarize and critique formal research reports; (b) developing abilities to prepare and present a scholarly subject professionally in front of an audience, i.e. group meeting, department seminar and so on.

Prerequisite

Willing to think quantitatively in biology, i.e. comfortable with college math, phys, and chem.
Grading Policy

Grade will be based on literature presentation and literature critique starting tentatively on the Tue of week 2 (Oct 6).

• Literature presentation, 65%, is a formal presentation of an assigned journal paper. Presentation is set to be 17 min (about 16 slides) and 8 min of questions. Please follow your summary outlines (see below) to prepare your presentations. Also remember to introduce the PI’s group and research interests before your paper presentation to make it more interesting. The time limit will be enforced. You will lose points if your talk is either too short (less than 15 min) or too long (over 20 min). Please practice to make sure you can make it within the allocated time. It’s also strongly recommended that you write a transcript to summarize what you want to say due to the time limit.

The student presentations will tentatively start on the Tue of week 2 (Oct 6), depending on how many students enroll at the beginning of week 1. I will assign graduate students to present first. These will be followed by presentations by undergraduates so you have a better idea how to present.

Past experiences show that we can only arrange two student presentations per lecture due to the long discussion and question time after each talk. Thus the class will be divided into four groups (up to 8 students per group so far) for easy management. Briefly two groups will present on either Tue/Thr so we will discuss four papers per week if there is no holiday or other issue. Since all four groups will present in turn – two groups per day, each group will only present once per week. The group assignment will be posted on Sept 29 (Tue), one week before the graduate students’ turns to present.

• Literature critique, 35%, is a weekly summary of an article assigned for your reading. If one of your group members is presenting on a given day of a given week, you are assigned to read the same paper to be presented. The students who are presenting are exempt from this assignment in that week. Following this schedule, you only need to read/turn in critique for one paper per week. We will make sure that each student reviews the same number of papers by the end of the quarter.

Given the enrollment status, each student will submit a minimum of seven summaries in this quarter. Note that presenters do not need to return
summaries for the papers to be presented. Some groups will have more than eight papers assigned. In this case, only seven summaries are required. For the extra paper, i.e. T#_9 paper where # is the group number, every student in the class is encouraged to submit a summary, which earns an extra 5% point, i.e. the total point for the literature critique will be increased to 40% from 35% when the extra summary is submitted.

The summary should highlight the following. (1) What is the biomedical significance of the research? (2) What is the specific question to be answered in the research? (3) How does the author approach the question? (4) What is the conclusion? (5) What is the scope or limitation of the conclusion? Use no more than 250 words in your summary. Also, prepare two questions that you can potentially ask the presenter.

• Classroom involvement in strongly encouraged. For each student presentation, every other student in the class is encouraged to ask questions, whether the presenter is from your own group or not. We will record how many times each student asks questions throughout the quarter. A student will get one tick letter grade bonus if she/he asks eight or more questions by the end of the quarter.

• Class attendance is mandatory: you can miss no more than two lectures throughout the quarter. If you decide to show up, you have to arrive at the room no more than 5 min late. Late arrival will be treated as absence. If you miss three lectures, your letter grade will be reduced by one tick; if you miss five lectures, your letter grade will be reduced by two ticks; and so on.

• There is no final exam. However the final exam time may be used for presentations if we run out of presentation time.

• Grades will not be curved. The grading scheme here is designed to be as fair as possible and honor your efforts as accurately as possible. Most students did great in our class in the past.

Suggested References

Molecular Modelling by Leach; Relevant chapters: 1, 4 - 9, 10, and 11. Students are encouraged to explore online for alternative reading materials.
Lecture Outline

• Review of biomolecules and biomolecular graphics (these are given as homework reading materials). Brief introduction to molecular interactions and molecular mechanics, molecular dynamics and Monte Carlo, solvation and electrostatics (these are covered in the first week).

• Biomolecular graphics using VMD will follow online tutorial at http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/index.html. The online tutorial will be left as homework to be finished by students at home before student literature presentations. Note that use of VMD generated graphics in your presentation will boost your presentation scores. This will be considered in assigning your presentation grade.

Class Logistics

• It is important to check email daily to make sure you don’t miss any announcements and assignments by email. Thus make sure your mailbox is not full and functions well throughout the quarter.

• Instructor’s presentation files and literatures will be posted on the class website before each lecture.

• You are required to finish a draft powerpoint file 48 hours before your presentation time and email the file to the instructor. This is to make sure you will be well prepared for your presentation. Note you have to practice for time as well and adjust your powerpoint file accordingly.

After the presentations, all final presentation files (both the powerpoint and the transcript if it’s not inside) will need to be emailed to the instructor as record for final grade assignment.