

## Syllabus Spring 2015

### BCM 484/684, Biomolecular Modeling

#### Lectures

Mo and We 10:35-11:30 AM LSC 215

Prof. Philip Borer

Office: 2-006 Sci Tech

Phone: 443 1835

Computer Lab

We TBD LSC 215

Dr. Deborah Kerwood

Office: 0-222D Sci Tech

Phone: 443 5925

The lectures and computer laboratory modules will emphasize practical experience in biomolecular modeling, connecting it with principles of structure, thermodynamics and kinetics. Students will learn to use computer programs for modeling large biomolecular structures. In addition they will learn principles of UV/Vis absorbance, fluorescence, and nuclear magnetic resonance spectroscopy, and x-ray diffraction as applied to biomolecular structure determination. The computer software programs to be used by students are widely used in pharmaceutical and biotechnology research and development.

A written report and oral presentation are required during the course (see time schedule). All students will take the midterm and comprehensive final exam (see time schedule for date and time). The final exam will have different questions for the graduate students and the undergraduates. Completion of molecular modeling projects designed by the student in consultation with the instructors will be required. Chimera, Amber, and other software will be discussed during the lab lecture and computational facilities will be available for use at specified times for student projects.

The prerequisite for BCM 484 is CHE 474, Structural and Physical Biochemistry. The prerequisite for BCM 684 is graduate standing and permission of the instructor.

#### Required text:

Tinoco, Sauer, Wang & Puglisi, *Physical Chemistry: Principles and Applications in Biological Sciences*, fifth ed., Prentice-Hall, ISBN-13: 978-0-321-88331-5. Instead of purchasing the hardcover text, an e-text is available at:

<http://www.mypersonstore.com/bookstore/physical-chemistry-principles-and-applications-in-biological-9780321883315>

#### Recommended text:

Any modern Biochemistry textbook, e.g., Berg, Tymoczko, & Stryer, *Biochemistry*, W.H. Freeman.

#### Disability and Academic Integrity:

If you believe that you need accommodations for a disability, please contact the Office of Disability Services (ODS), <http://disabilityservices.syr.edu/>, located in Room 309 of 804 University Avenue, or call (315) 443-4498 for an appointment to discuss your needs and the process for requesting accommodations. ODS is responsible for coordinating disability-related accommodations and will issue students with documented Disabilities Accommodation Authorization Letters, as appropriate. Since accommodations may require early planning and generally are not provided retroactively, please contact ODS as soon as possible.

Syracuse University sets high standards for academic integrity. Those standards are supported and enforced by students, including those who serve as academic integrity hearing panel members and hearing officers. The presumptive sanction for a first offense is course failure, accompanied by the transcript notation "Violation of the Academic Integrity Policy." Students should review the Office of Academic Integrity online resource "Twenty Questions and Answers About the Syracuse University Academic Integrity Policy." Additional guidance can be found in the Office of Academic Integrity resource: "What does academic integrity mean?"

<http://academicintegrity.syr.edu/what-does-academic-integrity-mean/>

TENTATIVE SCHEDULE FOR CHE 484/684 M, We 10:35-11:30 v. 1

Prof. Philip N. Borer [pnborer@syr.edu](mailto:pnborer@syr.edu)  
0-221C Sci Tech 443 5925

Dr. Deb Kerwood [djkerwoo@syr.edu](mailto:djkerwoo@syr.edu)  
0-222D Sci Tech 443 5932

Items in { } are projects for the {computer laboratory}.

The second Modeling Project will be described in a live 15-20 min talk illustrated by computer graphics.

Grading: Lab modules and homework 15%, Exams 30%, Modeling Projects 50%, Participation 5%  
Late work is penalized at 10% per day late. Deadlines are 5 PM according to computer date stamps.

**ASSIGNMENTS AND SPECIAL ITEMS ARE MARKED IN THIS FONT. SOME STUDENT PRESENTATIONS MAY OCCUR OUTSIDE NORMAL CLASS MEETING TIMES.**

1	Mo	12-Jan	Handouts, intro to modeling lab
2	We	14-Jan	PDB files, Chimera modules { <b>Assign</b> Lab Module 1 ( <b>LM1</b> ), Chimera and PDB, Start modeling lab}
3	Mo	19-Jan	No lecture (MLK Celebration)
4	We	21-Jan	Introduction to Biopolymer building { <b>LM1 due; Assign LM2</b> , Modifying files and viewing}
5	Mo	26-Jan	Simulating Inter and Intramolecular Forces
6	We	28-Jan	Simulating Inter and Intramolecular Forces { <b>LM2 due</b> }
7	Mo	2-Feb	Molecular Dynamics computations {Consultations on Modeling Project 1}
8	We	4-Feb	No lecture { <b>Assign LM3</b> , MD for Giberellic Acid}
9	Mo	9-Feb	No lecture
10	We	11-Feb	No lecture { <b>Work on MP1</b> }
11	Mo	16-Feb	Strategies for Energy Minimization and Dynamics
12	We	18-Feb	Strategies for Energy Minimization and Dynamics { <b>LM3 due</b> , Q&A on MP1}
13	Mo	23-Feb	UV/Vis absorbance spectroscopy (Read Tinoco, Ch. 13 [pp. 489-507]) {Work on MP1}
14	We	25-Feb	UV/Vis absorbance { <b>MP1 PAPER DUE</b> }
15	Mo	2-Mar	UV/Vis absorbance and circular dichroism (Read Tinoco, Ch. 13 [pp. 520-525])
16	We	4-Mar	<b>Midterm exam</b> - Modeling PDB files, theory of EM, MD simulations
17	Mo	9-Mar	No lecture (Spring Break)
18	We	11-Mar	No lecture (Spring Break)
19	Mo	16-Mar	Fluorescence and FRET (Read Tinoco, Ch. 13 [pp. 507-519])
20	We	18-Mar	Fluorescence and FRET { <b>Assign LM4</b> , Active site inhibitor of HIV-1 protease; Consultations on MP2}
21	Mo	23-Mar	No lecture - consultations on MP2
22	We	25-Mar	Nuclear Magnetic Resonance (Read Tinoco, Ch. 14 [pp. 539-567]) { <b>Submit Abstract for MP2</b> }

23	Mo	30-Mar	Nuclear Magnetic Resonance
24	We	1-Apr	Nuclear Magnetic Resonance { <b>LM4 due</b> ; Work on MP2}
25	Mo	6-Apr	Nuclear Magnetic Resonance
26	We	8-Apr	X-ray diffraction and structure (Read Tinoco, Ch. 15 [pp. 574-611]) { <b>Work on MP2</b> }
27	Mo	13-Apr	X-ray diffraction and structure
28	We	15-Apr	X-ray diffraction and structure { <b>Work on MP2</b> }
29	Mo	20-Apr	X-ray diffraction and structure
30	We	22-Apr	<b><u>{ORAL PRESENTATIONS OF MP2}</u></b>
31	Mo	27-Apr	<b><u>{ORAL PRESENTATIONS OF MP2}</u></b>

Fri 1-May to 4-May <b><u>COMPREHENSIVE FINAL EXAM</u></b> <b><u>(TAKE HOME) -- PICKUP 12 NOON 1-MAY, TURN IN 12 NOON 4-MAY</u></b>
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