BINF 6202 / 8202: Computational Structural Biology

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Note: Whenever you email me regarding the course, please put BINF6202 in the subject line so that I will not inadvertently delete your email without reading it.

Conditions of enrollment:
Prerequisite: basic proficiency in biochemistry.
Co-requisite: BINF 6202L (Computational Structural Biology Lab), 0 credits.

Course description: This course will cover: (a) the fundamental concepts of structural biology (chemical building blocks, structure, superstructure, folding, etc.); (b) software for visualization, visualization styles, publication quality images; (c) the hierarchical nature of biomacromolecular structure classification; (d) computational methods to evaluate and compare biomacromolecular structure; (e) inferring structure/function relationships from structure; and (f) computational prediction of protein and nucleic acid structure from sequence.

Learning Objectives: All students successfully completing this course should:
• Understand the fundamental building blocks of protein structures
• Knowledge of experimental methods for structure determination
• Demonstrate understanding of PDB file format
• Compare and contrast protein structure classification methods
• Knowledge of quality assessment methods for protein structures
• Demonstrate solid understanding of protein structure comparison methods
• Understand different protein structure prediction methods
• Knowledge of sequence- and structure-based function prediction methods

Academic integrity: All students are required to read and abide by the Code of Student Academic Integrity. Violations of the Code of Student Academic Integrity, including plagiarism, will result in disciplinary action as provided in the Code. Definitions and examples of plagiarism are set forth in the Code. The Code is available from the Dean of Students Office or online.¹ A set of links to various resources on plagiarism and how to avoid it is available at the UNC Charlotte Library website.² Take home message: DO NOT CHEAT!

Cell phones/pagers: Interruptions to class by cell phones will not be tolerated.

Instructional methods: This course will be based on a mix of traditional lecture format (using the blackboard) and PowerPoint presentations. All PowerPoint presentations will be available on the web at the course website.

Attendance: There is no attendance policy; however, I will be less willing to assist outside of class those students that do not attend.

¹ http://www.legal.uncc.edu/policies/ps-105.html
² http://library.uncc.edu/display/?dept=instruction&format=open&page=920

Course website: [http://coitweb.uncc.edu/~drlivesa/BINF6202.html](http://coitweb.uncc.edu/~drlivesa/BINF6202.html).

Time & Location:

Lecture: Tu/Th, 9:30 am to 10:45 am in Bioinformatics 301.
Lab: Tu, 2:00 to 3:15 pm in Bioinformatics 105.

Exam schedule: There will be two exams, tentatively scheduled for Thursday, September 25th and Thursday, November 20th. The final exam is scheduled for Thursday, December 11 from 8:00 to 10:30 am.

Grading (BINF 6101): Students enrolled in BINF 6202 will be evaluated in the following manner: 25% exam 1; 25% exam 2; 30% final exam; and 20% homework/lab assignments. Final grades will be based on 10% increments (i.e., 90-100% = A; 80-89% = B; 70-79% = C; < 70% = U). The final exam will be cumulative.

Grading (BINF 8101): Students enrolled in BINF 8202 will be evaluated in the following manner: 24% exam 1; 24% exam 2; 30% final exam; 18% homework/lab assignments; and 4% journal article summary. Final grades will be based on 10% increments (i.e., 90-100% = A; 80-89% = B; 70-79% = C; < 70% = U). The final will be cumulative.

The journal article summary is a 3-5 double-spaced page overview of a research article from the primary literature relevant to the course material. Please get prior approval for the paper that you wish to review. This is due anytime before the final exam.

Lab assignments: There will be, approximately, one or two lab assignments between exams. In many instances, the labs assignments will also include homework questions designed to reinforce the topics covered in lecture. The labs will expose you to standard implementations of the methods and give you opportunities to interpret their results from data that you generate. Most of the labs will focus on server implementations of the methods, so they can be done from anywhere.

Getting help: Office hours are by appointment. The course TA is Mr. Alvin Farrel.

Calculators: You are free to use any resources that you want on the homework assignments and classroom exercises. However, I will only allow basic scientific calculators during exams. Cell phone calculators, graphing calculators, and other devices with the capability to save information and have additional functionality programmed are absolutely NOT allowed. If you have a question about your device, please see me with it before the first exam.

Course outline:

- Topic 1: Introduction
- Topic 2: Amino acids
- Topic 3: Protein structure
- Topic 4: Structural visualization (software and styles)
- Topic 5: The Protein Data Bank
- Topic 6: Analysis of protein structures and quality assurance
- Topic 7: Structure determination (experimental methods)
- Topic 8: Data representation and structural classification
- Topic 9: Secondary structure assignment
- Topic 10: Automated domain identification
- Topic 11: Structural superposition
- Topic 12: Protein structure alignment
- Topic 13: Secondary structure prediction
- Topic 14: Tertiary structure prediction – homology modeling
- Topic 15: Tertiary structure prediction – fold recognition and fragment assembly
- Topic 16: Contact order and protein folding kinetics
- Topic 17: Protein functional site prediction
- Topic 18: Protein design (the inverse folding problem)