SYLLABUS – CHEM 337 – COMPUTATIONAL STRUCTURAL AND CHEMICAL BIOLOGY

Course Description:
Theoretical and practical aspects of protein sequence alignments, secondary structure prediction, comparative modeling, protein-protein and protein-ligand docking. Structure-based drug design, virtual screening, quantitative structure activity relations, cheminformatics, and pharmacophore mapping in therapeutic development. This course includes a laboratory section.

Prerequisite:
Undergraduate students wishing to take CHEM 337 for credit must complete CHEM 231 first.

Instructor:
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Class:
T+Th 8:10a-9:25a, MRBIII 5131 and T 1:10p-4:00p SC 5119

Office Hours:
T+Th 9:30a-11:00a and by appointment

Course Materials:
All course materials including lecture notes, homework assignments, grades, and announcements can be found online at blackboard: oak.vanderbilt.edu

Grading:
First exam (25%), Second exam (25%), Homework (25%), Class and laboratory participation (25%). You can expect to receive a grade of A or A– for a semester average at or above 90%; semester averages below 50% will be assigned a grade of F.

Exams:
Both exams will have a concept and a problem component. If you have any conflicts with the dates of any of the exams, you must notify me within the two weeks of the start of the semester.
The Second Exam will be comprehensive. Before both exams there will be two lectures for summary, questions, discussion, recapitulation.

**Homework:**

There is typically one homework assignment per week. Homework is always due one week after its assignment. No late submissions will be accepted. No make-up homework will be given. There will be no homework during the week of exams. Homework solutions will be briefly discussed in class if major problems occurred or if requested by students.

**Laboratory:**

In the additional weekly practice time the protein structure prediction techniques discussed in the lecture will be practiced by executing tutorials. Students are encouraged to bring appropriate computational problems from their own research projects.

**Note on the Honour Code:**

All exams and homework assignments are on the Vanderbilt Honour System. You are permitted and encouraged to work in groups to work out the answers to the suggested problems; this is not a violation of the Honour Code. But, graded homework problems and exams should be answered without any outside help. A full description of the Honour Code is provided in the Vanderbilt University Student Handbook.

**Course Timetable (subject to adjustments):**

Aug 25: Lecture 01: Course Overview and Introduction to Protein Structure

Aug 30: Lecture 02: Sequence-Sequence Alignment Methods
  *Laboratory: Introduction to Linux, Protein Structure & Interactive Molecular Graphics*

Sep 01: Lecture 03: Sequence Based Secondary Structure Prediction

Sep 06: Lecture 04: Protein Family Classification through Hidden Markov Models
  *Laboratory: Sequence-Sequence Alignment and Secondary Structure Prediction*

Sep 08: Lecture 05: Fold Recognition & Sequence-Structure Alignment (Threading)

Sep 13: Lecture 06: Comparative Modelling and the Loop Closure Problem
  *Laboratory: Fold Recognition & Sequence-Structure Alignment*

Sep 15: Lecture 07: De Novo Protein Structure Prediction

Sep 20: Lecture 08: Modeling Protein Side Chains from Rotamer Libraries
  *Laboratory: Comparative Modeling & Loop Closure*

Sep 22: Lecture 09: Protein Structure Determination from Limited Experimental Datasets

Sep 27: Lecture 10: Protein Design
Laboratory: De Novo Protein Structure Prediction
Sep 29: Topic Overflow, Summary, First Exam Preparation

Oct 04: Topic Overflow, Summary, First Exam Preparation  
Laboratory: Modeling Protein Side Chains from Rotamer Libraries and Protein Design
Oct 06: Fall Break

Oct 11: First Exam  
Laboratory: Topic Overflow if needed
Oct 13: First Exam Results

Oct 18: Lecture 11: Structure-Structure Alignment Techniques and Fold Classification  
Laboratory: Structure-Structure Alignment & Fold Classification
Oct 20: Lecture 12: Protein-Protein-Docking

Oct 25: Lecture 13: Protein-Ligand-Docking  
Laboratory: Protein-Protein-Docking and Protein-Ligand-Docking
Oct 27: Lecture 14: Structure-based Virtual Screening & Drug Design

Nov 01: Lecture 15: Constitution, Configuration, & Conformation  
Laboratory: Structure-based Virtual Screening
Nov 03: Lecture 15: Constitution, Configuration, & Conformation

Nov 08: Lecture 16: Structure Generators  
Laboratory: Quantitative Structure Activity & Property Relations
Nov 10: Lecture 17: Molecular Descriptors

Nov 15: Lecture 18: QSAR, Ligand-based Virtual Screening, and Pharmacophore mapping  
Laboratory: Ligand-based Virtual Screening
Nov 17: Lecture 18: QSAR, Ligand-based Virtual Screening, and Pharmacophore mapping

Nov 22: Thanksgiving
Nov 24: Thanksgiving

Nov 29: Topic Overflow, Summary, Second Exam Preparation  
Laboratory: Pharmacophore mapping
Dec 01: Topic Overflow, Summary, Second Exam Preparation

Dec 06: Second Exam  
Laboratory: Topic Overflow if needed
Dec 08: Second Exam Results and Grades