UTTyler SCHOOL OF MEDICINE

BIOT 5221L **Proteins & Nucleic Acids - LAB** **Credit Hours: 2**

Semester: Spring **Year:** 2023
Class Day/Time: Mondays, 1:30-5:30p **Class Location:** D247; Hudnall Auditorium

Instructor of Record: Dr. Pierre Neuenschwander Professor
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Office Hours: Any time arranged by email.

Course Description: The goal of the course is to provide a critical understanding of the relationship between structure and function of biological macromolecules such as proteins and nucleic acids. The Lab component of this course will give the students hands-on experience in using molecular modeling programs to learn how to manipulate protein structures, performing docking simulations, and graphically display proteins and nucleic acids structures.

Prerequisite: BIOT 5312 **Co-requisite:** BIOT 5221

Goals of Course & Course Objectives:

Course Objectives:

1. To be able to communicate and discuss fundamental molecular biochemical principles pertaining to protein structure & function.
2. To be able to use molecular modeling and molecular docking tools.
3. To be able to find and process scientific information.
4. To be able to explain and present molecular graphics.

Student Learning Outcomes (Course Competencies):

1. The student will be able to describe molecular modeling and its uses in biotechnology.
2. The student will be able to generate a polypeptide *in silico* and manipulate its structure.
3. The student will demonstrate their ability to use molecular modeling software such as *PyMol*, and *AutoDock Vina*.
4. The student will be able to access, download and visualize x-ray crystal structures of molecules from the RCSB Protein Data Bank.
5. The student will be able to perform *in silico* mutagenesis studies as well as *in silico* docking studies of various molecules.
6. The student will be able to discuss properties of protein structure and ligand interactions.

Subject-specific skills:
Students will learn how to use computer modeling and docking programs to perform in-silico experimentation and mutational studies.

Course Assessment/Methods of Evaluation:
Students who successfully complete the lab portion of this course will demonstrate a thorough understanding of protein structure, function, and binding interactions.

- Class Participation and Attendance (20% of final grade): Punctual attendance is critical. There will be a sign-up sheet for each class and it will be mandatory to sign in (legibly) for each class to record your attendance. Students are expected to be in attendance for the majority of class time to receive full credit. Each class will have an attendance credit total of 2 points. Tardiness of more than 30 minutes will result in a reduction of 1 attendance credit for that class, with an equivalent reduction after 60 min.
- Assignments & Quizzes (30% of final grade): There will be several assignments and Quizzes in this course, each will be worth from 10 to 20 points.

- Projects (50% of final grade): Each of the two major projects (Midterm and Final) will be worth 25% each.

Attendance	= 20%
Assignments	= 30%
Final Project	= 25%
Midterm Project	= 25%
Total	**= 100%**

Each person's total score in each category will be divided into the maximum possible score for that category and then multiplied by the fractional percentage. These will be summed to obtain your final grade. For example:

[(29/30)*0.2] + [(35/40)*0.3] + [(90/100)*0.25] + [(95/100)*0.25] = 0.918 = 92% = A
[*Attendance*] + [*Assignments*] + [*Midterm Project*] + [*Final Project*]

Linked Program Learning Outcomes:
The student learning outcomes listed above address the following Biotechnology Program PLOs:

- PLO-2. The student will demonstrate mastery of basic and advanced biotechnology methods
- PLO-3. The student will demonstrate the ability to safely operate basic and advanced laboratory equipment, analytic devices and computers.
- PLO-4. The student will demonstrate independent and critical thinking skills integrated with the ability to utilize multiple informational resources.

Textbook:
None.

Course Content:
Topical Content:

- Use of computers in biomolecular modeling
- How computers predict structures
- How computers display x-ray diffraction data
- Using computers in drug discovery
- Visualizing biomolecules
- Constructing biomolecules *in-silico*
- *In-silico* mutational studies
- *In-silico* docking simulations
- From *in-silico* to *in-vitro:* Testing the hypothesis

Programs that the students will become familiar with and proficient in:

- *PyMol*
- *Autodock Vina*
- *MC-Fold and MC-Sym*

Tentative Schedule:

Week 1. Introduction and Course Overview (1/9/2023). We will go over some background (review) and present a brief overview of the course. Then we will spend some time learning how to access the VPN and move files back and forth in preparation for the next lab class.

Week 2. Introduction to *PyMOL* (1/16/2023). **MLK Holiday so no in-class meeting today**. Read through the *PyMol for the Beginner* lesson on *CANVAS* and then take the **PyMol Quiz** before the next class.

Week 3. Building a Polypeptide (1/23/2023). Read the two papers in *CANVAS* for consideration and discussion during class: What is the difference between the "helix propensity" and the "hydropathy index"? Are they related? (we will discuss in class). After the discussion, we will build your first molecular model (a peptide) using *PyMOL*.

Week 4. *AutoDock* (1/30/2023). Docking molecules with *AutoDock Vina*. You will need to go through the *CANVAS* lessons *Using AutoDock and AutoDock Vina* and then take the ***AutoDock* quiz** before class. In lab we will prepare your molecular docking partners for the docking procedure as well as prepare your configuration file. These will be submitted to me at the end of class so I can review them before next class.

Week 5. Stampede2 on TACC (2/6/2023). Today you will set up your account on TACC and I will add you to the docking allocation for the class. We will review how to access and use the TACC resources. You will also learn some simple Unix commands so that you can move around within the supercomputer using command line. If time permits we will also learn how to transfer files between the VPN computer and the supercomputer as well as log into the supercomputer and execute some commands to setup the system for next week.

Week 6. Set up a Docking Run (2/13/2023). Today you will submit your first docking project to the supercomputer. It will involve setting up your "batch script" based on the template in this section. The batch script has nothing to do with docking but has all the required commands that the supercomputer will need to know what to do and set up the docking run for you and send the proper docking command to *Vina*. Once you have submitted the job, it is just a matter of waiting in the "queue" for the job to be completed. Depending on how many people are using the supercomputer at the time, this can be anywhere from a few minutes to 24 hours. We will review the docking results next week unless all of us get our results back today. We will see how it goes.

Week 7. Analyzing Your First Docking Project (2/20/2023). Today you will download the docking results from your docking run and analyze the structures (molecular poses) on *PyMOL*. You will generate some figures of the results and write it all up in a short lab report (using the **Short Lab Report Template**) and submit it using the link in *CANVAS*. If we were able to download and analyze docking results last week, I will give you another molecule to dock today for extra practice. Either way, the peptide docking results are to be written up as a short lab report and submitted by next week.

Week 8. Start on Your Midterm Project (2/27/2023). Choose a molecular pair for your midterm and begin your study. The completed **Midterm Lab Report** is due on March 20 by 5:00 pm. Use the Midterm Project link in *CANVAS*.

Week 9. Analyzing Your Docking Results for Your Midterm Project (3/6/2023). Complete work on your Midterm docking study and Lab Report.

Week 10. Spring Break (3/13/2023). No Lab class. Work on your own on Midterm project.

Week 11. *MC-Fold* and *MC-Sim* (3/20/2023). We will start a new module this week and learn how to fold an RNA molecule into different structures (folding patterns) and generate 3-D structures from these folding patterns. The lab is all through *CANVAS* this week. It will involve you working on your own (or in groups, however you like) to go through the lesson. You will need to have two windows open on your monitor: One with the lesson, and the other one with a web browser to access yet another supercomputer (this one is at the University Montreal). This lesson will likely take the entire lab time and perhaps longer.

Week 12. RNA Folding Project (3/27/2023). Since the "Relieving" command takes so long, you likely will not have been able to see the completed results last week. It should have been working all this time if you kept your window open and hopefully, by now it is finished. But some of you who forgot to keep the window open the entire time may have lost your work and will need to re-do it. Today is the day to catch up and get to the point where all of you have relieved structures to analyze. We will perform a Cluster Analysis of these relieved structures to generate a more manageable number of structural families.

Week 13. Finishing up and Reviewing the Results of the Folding Experiment (4/3/2023). Mostly a time to catch up and finish this module before starting on your final projects next week.

Week 14. Start Your Final Project (4/10/2023). Details will be given during class but the project will involve starting from an RNA sequence, folding and making 3D-structural predications, performing a cluster analysis to identify families, and docking a representative from each family to a protein target. You will have until Finals Week to complete this and submit your lab report Final Project write up.

Week 15. Continue work in lab on your Final Project (4/17/2023).

Week 16. Final Project due no later than Wednesday April 26, 2023, at 5:00 pm.

Other Class Policies:

Attendance:

Regular or punctual attendance is expected. If a student misses a class or lab, the student is responsible for obtaining any information distributed during those times. Make-ups are possible only under certain instances. Arrangements for any make-ups and/or missed labs should be discussed directly with the instructor for that day's class.

Academic Honesty:

Any student who commits an act of scholastic dishonesty is subject to discipline. Scholastic dishonesty includes, but is not limited to, cheating, plagiarism, collusion, the submission for credit of any work or materials that are attributable in whole or in part to another person, taking an examination for another person, any act designed to give unfair advantage to a student or the attempt to commit such acts.

Cheating

Dishonesty of any kind involving examinations, assignments, alteration of records, wrongful possession of examinations, and unpermitted submission of duplicate papers for multiple classes or unauthorized use of keys to examinations is considered cheating. Cheating includes but is not limited to:

- Using or attempting to use unauthorized materials to aid in achieving a better grade on a component of a class.

- Falsifying or inventing any information, including citations, on an assigned exercise.
- Helping or attempting to help another in an act of cheating or plagiarism.

Plagiarism

Plagiarism is presenting the words or ideas of another person as if they were your own. Materials, even ideas, borrowed from others necessitate full and complete acknowledgment of the original authors. Offering the work of another as one's own is plagiarism and is unacceptable in the academic community. A lack of adequate recognition constitutes plagiarism, whether it utilizes a few sentences, whole paragraphs, articles, books, audio-visual materials, or even the writing of a fellow student. In addition, the presentation of material gathered, assembled or formatted by others as one's own is also plagiarism. Because the university takes such misconduct very seriously, the student is urged to carefully read university policies on Misconduct in Research and Other Scholarly Activity 05.00. Examples of plagiarism are:

- Submitting an assignment as if it were one's own work when, in fact, it is at least partly the work of another.
- Submitting a work that has been purchased or otherwise obtained from an Internet source or another source.
- Incorporating the words or ideas of an author into one's paper without giving the author due credit.

Adding/Dropping:

The official deadline for adding and dropping courses is as published in the academic calendar (Registrar Withdrawal webpage). However, students are strongly encouraged to meet with their graduate advisor or the Program Coordinator prior to adding/dropping courses. Movement into and out of classes after the 4th class day requires approval of the Program Director. Each student is responsible for their own enrollment status with the university.

Disability Accommodations:

UT Tyler HSC abides by Section 504 of the Rehabilitation Act of 1973 and the Americans with Disabilities Act, which mandate reasonable accommodations be provided for students with documented disabilities. If you have a disability and may require some type of instructional and/or examination accommodations, please contact me early in the semester so that I can provide or facilitate provision of accommodations you may need. If you have not already done so, you will need to register with the Student Services Office (located on the main campus). You may call 903-566-7079 for more information.

Program:	Master of Science in Biotechnology
Degree:	MS
Department:	Cellular and Molecular Biology
School:	Medical Biological Sciences
Course:	**BIOT5211/5221L – Proteins and Nucleic Acids** (and associated lab)

Area	Marketable Skill*
TASKS	Maintain accurate laboratory records and data.
	Design molecular or cellular laboratory experiments, oversee their execution, and interpret results.
TECHNOLOGY SKILLS	Analytical or scientific software, Graphics and molecular imaging software – PyMOL, Autodock Vina, MGL Tools
	Object or component-oriented development software - Autodock Vina, MGLTools, Unix commands in supercomputer environment
SKILLS	**Critical Thinking** — Using logic and reasoning to identify the strengths and weaknesses of alternative solutions, conclusions, or approaches to problems.
ABILITIES	**Written Comprehension** — The ability to read and understand information and ideas presented in writing.
	Inductive Reasoning — The ability to combine pieces of information to form general rules or conclusions (includes finding a relationship among seemingly unrelated events).
	Written Expression — The ability to communicate information and ideas in writing so others will understand.
WORK ACTIVITIES	**Analyzing Data or Information** — Identifying the underlying principles, reasons, or facts of information by breaking down information or data into separate parts.
	Updating and Using Relevant Knowledge — Keeping up-to-date technically and applying new knowledge to your job.
	Getting Information — Observing, receiving, and otherwise obtaining information from all relevant sources.
	Documenting/Recording Information — Entering, storing, or maintaining information in written or electronic/magnetic form.
	Processing Information — Compiling, coding, calculating, tabulating, or verifying information or data.

*All marketable skills listed for this course and program were drawn from the Knowledge, Skills, and Abilities identified by the US Department of Labor and Statistics for “Biological Technicians” and “Molecular and Cellular Biologists” as published on O*Net Online (www.onetonline.org)