Instructor of Record: Dr. Pierre Neuenschwander
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Office Hours: Mondays 12pm-1pm. 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:

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[(29/30)*0.2] + [(35/40)*0.3] + [(90/100)*0.25] + [(95/100)*0.25] = 0.918 = 92% = A
\]

**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 modeling
- How computers predict structures
- How computers display x-ray diffraction data
- Using Computers in drug discovery
- Visualizing molecules
- Constructing molecules \textit{in-silico}
- \textit{In-silico} mutational studies
- \textit{In-silico} Docking simulations
- From \textit{in-silico} to \textit{in-vitro}: Testing the hypothesis

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

- \textit{PyMol}
- \textit{Autodock Vina}
- \textit{MC-Fold and MC-Sym}

**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 and Graduate Bulletin (typically the day before Census Day). 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. Students can drop until mid-semester without a WP or WF. Drops after mid-semester require approval of the Dean. Each student is responsible for their own enrollment status with the university.

Disability Accommodations:
UTHSCT 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 UT Tyler Campus). You may call 903-566-7079 for more information.