January 22, 2022

Syllabus: BIOSC 1640: Computational Biology Research

January 22, 2022

General Information

Instructor

Instructor: Jacob D. Durrant
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Class Description

Students will use computational-biology methods to address an authentic research question. The course goal is to further expose students to the basic principles of computational structural biology. Students will learn through lectures taught by Dr. Durrant and a hands-on group project. The project will allow students to apply the relevant tools and demonstrate their acquired knowledge.

Schedule

Lectures and group work sessions are on Fridays, from 1:00 to 3:30 PM, in 1500 Wesley W. Posvar Hall, except for those weeks when university classes are held remotely due to the pandemic. Students should always bring a laptop computer to class. **If you don't have a laptop, speak with me during the first week.** If necessary, you might consider checking out a laptop from Hillman Library. The schedule below (Table 1) may change based on the class's needs/interests/pace. Always consult Canvas for an up-to-date syllabus.

Table 1: Lecture schedule (subject to change).

Date	Lecture Topic	Assignment(s) Due
01-14-21	Syllabus, drug discovery, characteristics of a good drug target, Protein Data Bank, Google Scholar	
01-21-21	Docking, Webina	Individual: Select protein drug target, and writeup
01-28-21	Scientific writing	Individual: Find Webina parameters to recapture the crystallographic pose, and writeup
02-04-21	Cheminformatics, similarity searching, PubChem, drug-like properties	Group: Select protein drug target for the group
02-11-21	Protein/ligand interactions, BINANA	Individual: Select five molecules that are chemically similar to a known ligand, and writeup Group: "Introduction" draft
02-18-21		Group: Compile all group members' molecules Group: Beginning of "Materials and Methods" and "Results" drafts
02-25-21	TBD	Individual: Dock your molecules into the protein, characterize the predicted protein/ligand

		interactions, and writeup
03-04-21	Lead optimization, DeepFrag	Group: Compile all group members' docking runs and interaction analyses Group: Updated "Materials and Methods" and "Results" drafts
03-11-21	Spring Break	
03-18-21		Group: Mid-term presentations Group: Compiled and updated written document with all sections, references, etc.
03-25-21		Individual: Use DeepFrag to optimize two of your ligands, and writeup Individual: Peer feedback on other group's compiled document
04-01-21	TBD	Group: Collect all group member's optimized ligands Group: Updated "Materials and Methods" and "Results" drafts
04-08-21	TBD	
04-15-21	Invited career speakers	Group: Final written reports
04-22-21		Group: Final presentations

Lectures are unlikely to take the entire 2.5 hours, and some class periods may not have lectures. Once the lecture finishes, students should get together with their groups and work on their projects or homework assignments.

- Start by discussing what your group accomplished this past week. What went well? What could go better?
- Make a detailed plan describing what you will accomplish next week, dividing the tasks among your group members.
- Present your accomplishments and plan to the class (five minutes), get feedback.
- Begin working on the tasks together. You may need to meet outside of class to finish the week's work.

I will also be available during this time should you have any questions about the project goals, how to do the homework assignments, how to use key online resources, how to perform relevant techniques, etc. Participating in after-lecture group and classroom discussions will likely be critical for success.

Assignments

Scores on individual assignments and group written reports/presentations will determine final grades. If circumstances require us to reschedule any assignment due dates, I will update the syllabus on Canvas. It is the students' responsibility to consult the latest version of the syllabus to verify all

due dates.

Group Project (50% of final grade)

Groups of roughly six students will work together on group projects. The overall goal of these projects is to identify small molecules that might bind to a disease-relevant protein target, modifying its activity in a way that could benefit human health.

Written Research Report

Submitting documents for evaluation. Each written document (e.g., draft, final report, etc.) is due at the beginning of class. I may not accept documents turned in after that time unless you provide a documented reason outside of your control. I also reserve the right to deduct points for late submissions. Don't forget to include the FULL names of all group members beneath the project title. Every time you email me a report section, start the subject line with "BIOSC 1640:".

Students must submit documents in Microsoft Word (DOC or DOCX) formats. Documents written using other word processors should be converted to Word formats before sending them to me. Documents sent in other formats may be returned. Students who do not use an appropriate format may be penalized.

All group members should participate equally. Every time your group turns in a draft or final version of the written report, each group member should send me a separate, confidential email with a "percent effort" evaluation. The email should include a list of all group members and your personal assessment of the percent effort (meaning writing + research) that each contributed to the assignment. I will take these confidential emails into account when grading the group assignments. If the group feels that one of its members is not contributing to the project, please talk to me as soon as possible. Every student must contribute substantially to every section of the document. It is not acceptable, for example, for one group member to write the *Introduction* section and another to write the *Results and Discussion*.

Be sure to consult the Group Project Guide. The guide provides further details regarding the required content and formatting.

Group Presentations

Group presentation details. All group members should participate. The presentation slides should cover the same material covered in your final written project, with a similar organization. Be sure to answer the same questions in the oral presentation that I asked you to answer in the final written report (see the Group Project Guide). A question-and-answer session will follow each presentation. Be sure to email me a copy of your slides afterward.

Be sure to consult the Group Project Guide. The guide provides further details regarding the required content and formatting.

Individual Assignments (50% of final grade)

Homework Assignments

Each student should turn in homework assignments separately (i.e., not as a group). These assignments should include only each student's own work, but students are encouraged to consult with one another to understand the relevant concepts and techniques. Homework assignments

provide the data that will ultimately be incorporated into the group research report and presentations, so group members may wish to discuss their respective assignments with each other. I will post each assignment to Canvas the week before it is due.

Peer Review Assignments

Each student will independently and individually edit a draft of another group's written report. Turn in a copy with only your peer-review edits (i.e., do not merge your edits with anyone else's into the same document). For all peer-review assignments, students will be graded individually rather than as groups.

Edit for brevity, clarity, formatting, references, grammar, tone, etc. Be thorough in your edits. This assignment requires more than just reading over the report and saying, "it looks good." The goal is to practice scientific-editing skills, which are critical in many bioscience jobs.

Track all your changes so I can review them. Tracking changes will also help the original authors better understand how to improve. Add a new section entitled "Reviewer" to the document you're editing and place your FULL name in this section. Creating this separate section is critical to distinguish between those who originally wrote the document and the person who edited it.

Grading Policies

Final Grade

I will assign letter grades according to the following scale: A (≥94%), A- (≥90%), B+ (≥86%), B (≥83%), B- (≥80%), C+ (≥76%), C (≥73%), C- (≥70%), D+ (≥66%), D (≥63%), D- (≥60%), F (<60%).

For clarity's sake, I will post a spreadsheet describing how much I expect each individual and group assignment to contribute to the final grade, but this spreadsheet is not final or binding. If necessary, I reserve the right to modify each assignment's contribution to the final grade. For example, I may curve the grading scheme to benefit the class if it's appropriate. I also reserve the right to provide extra-credit points.

Withdrawal Policy

If you cannot stay current with the material, regardless of the reason, consider withdrawing from the course. Please consult the official academic calendar to learn when the add/drop period ends and when the monitored withdrawal form must be submitted to the Dean's Office.

G Grades

In some rare cases, extenuating personal circumstances arising after the withdrawal deadline may prevent a student from finishing the course. Per SAS guidelines, if such students have been attending the course and making regular progress, they may petition for a G grade (University of Pittsburgh Undergraduate Bulletin, 1999-2002, p.29). If you find yourself in this situation, send me a request in writing that documents your reason(s) for the grade-change request. You will have to complete the coursework before the G grade can be removed.

Course Materials

Required Materials

This course does not require a textbook. I will post links to online resources, articles from the scientific literature, etc., to support what we discuss in class.

Course Website

Course materials and an up-to-date syllabus will be available through Canvas.

Additional Information and Resources

COVID-19 Precautions

During this pandemic, it is extremely important that you abide by the public health regulations, the University of Pittsburgh's health standards and guidelines, and Pitt's Health Rules. These rules have been developed to protect the health and safety of all of us. Universal face covering is required in all classrooms and in every building on campus, without exceptions, regardless of vaccination status. This means you must wear a face covering that properly covers your nose and mouth when you are in the classroom. If you do not comply, you will be asked to leave class. It is your responsibility to have the required face covering when entering a university building or classroom. For the most up-to-date information and guidance, please visit coronavirus.pitt.edu and check your Pitt email for updates before each class.

If you are required to isolate or quarantine, become sick, or are unable to come to class, contact me as soon as possible to discuss arrangements.

Classroom Recording

Students may not record classroom lectures, discussions, and activities without my written permission. Any recordings I approve must only be used by the authorized student for their private use.

Academic Integrity

Cheating/plagiarism will not be tolerated. Students suspected of violating the University of Pittsburgh Policy on Academic Integrity will be required to participate in the outlined procedural process as initiated by the instructor. A minimum sanction of a zero score for the homework, exam, or presentation will be imposed.

Students agree that by taking this course, all required papers may be subject to plagiarism detection using iThenticate or some other automated system. All submitted papers may be included as source documents in the iThenticate (or other) reference database to detect plagiarism of such papers.

Disability Resources

If you have a disability for which you are, or may be, requesting an accommodation, you are encouraged to contact both the instructor for this course and the Office of Disability Resources and Services, 140 William Pitt Union, 412-648-7890/412-624-3346 (Fax), as early as possible in the

term. Disability Resources and Services will verify your disability and determine reasonable accommodations for this course.

Email Communication

Each student is issued a University email address (username@pitt.edu) upon admittance. This email address may be used by the University for official communication with students. Students are expected to read email sent to this account on a regular basis. Failure to read and react to University communications in a timely manner does not absolve the student from knowing and complying with the content of the communications. The University provides an email forwarding service that allows students to read their email via other service providers (e.g., Hotmail, AOL, Yahoo). Students that choose to forward their email from their pitt.edu address to another address do so at their own risk. If email is lost as a result of forwarding, it does not absolve the student from responding to official communications sent to their University email address. To forward email sent to your University account, go to http://accounts.pitt.edu, log into your account, click on Edit Forwarding Addresses, and follow the instructions on the page. Be sure to log out of your account when you have finished.