UC San Diego
BIOLOGICAL SCIENCES

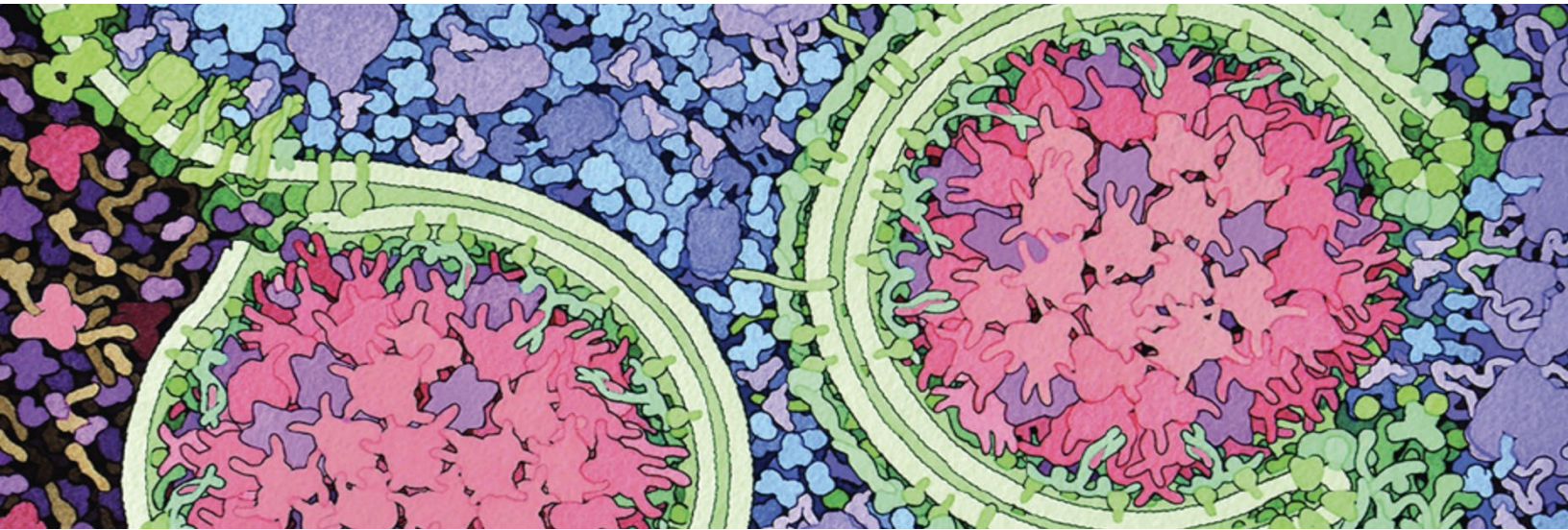# BIBC 194-Structural Biochemistry

Spring 2024

Lecture Time: in person most days & zoom all days, in 2622 York Hall, Tu 12:00 -1:20 pm
Instructor: Rommie Amaro
Email: ramaro@ucsd.edu
Office Hours: Fridays 2-3 pm
Course Website: https://canvas.ucsd.edu/courses/54428

Welcome!

I am looking forward to being your instructor for this quarter and my main goal is to teach you the course material and introduce you to modern approaches in computational structural biology. This is a seminar course that will take place at a high level; your grade will be based on your participation and weekly written assignments.

Instructor communication policy: I am available to meet with you during in-person lectures, office hours, or by email. If you have questions, I encourage you to attend office hours as it's easier to explain concepts in person. Due to volume, mail replies will be limited to 1-2 sentences in most cases. For emergencies, please contact me via email by writing BIBC194 as the subject and if I do not respond within 48 hours, please send me a reminder email. I will do my best to be responsive on the weekends, but I am human taking care of four kids and need down time too. Let's make this a great quarter!

Course Description

Computational Structural Biology is undergoing a revolution, thanks to increased experimental datasets, algorithmic advances, and continually evolving computer hardware. For example, AlphaFold made real the promise and use of artificial intelligence (AI) methods to enormous gain for the scientific community. In parallel, molecular, subcellular, and cell-scale simulations use, integrate, and extend experimental datasets providing novel hypotheses and views into regions of time and space that are otherwise inaccessible to experiment. This course will cover an overview of modern computational structural biology methods, through reading, discussing, and presenting primary literature.

Student Learning Outcomes:

By the successful completion of this course, you will be able to understand:

- AlphaFold and other computational methods to determine biological structure
- MD simulations at the molecular and mesoscale levels
- Analysis methods & application for cryoEM and cryoET
- Protein design methods & applications
- Antibody / immunogen design methods & applications
- Protein-ligand docking

Course Objectives:

We will review and discuss modern literature, focusing on novel and emerging methods in computational structural biology.

Course Format:

- **Lectures:** Lectures will be held in person (most days) and by zoom (always), and will be recorded via UCSD's videocast system. **Attendance in our weekly course sessions is essentially mandatory, as your grade is based on participation.** Expect questions and extensive discussion of the papers to be discussed in our weekly sessions.

- **2 lectures will be ZOOM ONLY:** Due to an unavoidable scheduling conflict, two lectures of the term (April 2 and May 7) will be offered ONLY BY ZOOM. All other sessions will be held in-person (but also live broadcast by zoom) in the scheduled lecture hall. The ZOOM-ONLY days are listed in the schedule, marked with ZOOM after the day.

Course Materials and Tools:

- There are no textbooks for this course. We will read and review the primary literature.
- Technology Requirement and Support
  - A computer equipped with video and mic.
  - Access to the internet.
- Accessing Canvas
  - https://coursefinder.ucsd.edu/
  - Login: UC San Diego Active Directory credentials

Grading & Assessment

This is a high level course which is based on participation. You will receive a grade for attendance and participation.

Schedule of Learning Modules:

Week	Lectures	Topic	✔
1	L1: T 4/2 **zoom**	Introduction of course/Overview	
2	L2: Tu 4/9	AlphaFold & AlphaFold Multimer	
3	L3: Tu 4/16	D3R Grand Challenge 4, DiffDock, & Posebusters	
4	L4: Tu 4/23	CryoEM: ModelAngelo, ManifoldEM	
5	L5: Tu 4/30	MD Simulations- molecular: Beyond Shielding, GlycanGate	
6	L6: Tu 5/7 **zoom**	MD Simulations - mesoscale: AI-Driven Multiscale Simulations…, Breathing & Tilting	
7	L7: Tu 5/14	CryoET: Review paper by Engel & colleagues, Villa et al. nuclear pore basket	
8	L8: Tu 5/21	Protein Design: Review by Kortemme, RASP by Lindorff-Larson, RosettaFold	
9	L9: Tu 5/28	Antibody / immunogen design: simulation-driven design paper by Amaro, de novo design paper by Baker	
10	L10: Tu 6/4	Interesting AI papers for dynamics	
11			

Student Resources for Support and Learning

- **Library Help**

    For questions about eReserves and research tools:

    https://library.ucsd.edu/ask-us/triton-ed.html

- **Learning Resources**

    Writing Hub

    Supplemental Instruction

    Tutoring

    Mental Health Services

- **Community Centers**

    Learn about the different ways UC San Diego explores, supports and celebrates the many cultures that make up our diverse community. https://students.ucsd.edu/student-life/diversity/index.html

- **Accessibility**

    Students requesting accommodations for this course due to a disability must provide a current Authorization for Accommodation (AFA) letter issued by the Office for Students with Disabilities (OSD) which is located in University Center 202 behind Center Hall. Students are required to present their AFA letters to Faculty (please make arrangements to contact me privately) and to the OSD Liaison in the department in advance so that accommodations may be arranged.

    Contact the OSD for further information: https://disabilities.ucsd.edu/.

    osd@ucsd.edu | 858. 534.4382

- **Inclusion**

I am committed to creating a learning environment that supports diversity of thought, perspective, experience, and identity. This will be key to our success. Science is all about pooling insight and seeing problems from as many perspectives as possible. So, please share your thoughts.

 I am also open to anonymous feedback am fully willing to facilitate it.

Office of Equity, Diversity, and Inclusion:

858.822.3542 | diversity@ucsd.edu | https://diversity.ucsd.edu/

https://students.ucsd.edu/student-life/diversity/index.html

https://regents.universityofcalifornia.edu/governance/policies/4400.html

- **Basic Needs**

    Any student who has difficulty accessing sufficient food to eat every day, or who lacks a safe and stable place to live, and believes this may affect their performance in this course, is encouraged to contact:

    foodpantry@.ucsd.edu | basicneeds@ucsd.edu | (858)246-2632

- **Technical Support**

    For help with accounts, network, and technical issues:

    https://acms.ucsd.edu/contact/index.html

    For help connecting to electronic library resources such as eReserves and e-journals:

    https://library.ucsd.edu/computing-and-technology/connect-from-off-campus/

UC San Diego Academic Policies

- **ADMINISTRATIVE QUESTIONS**

    To drop/add a class or with other similar questions/issues, please contact the Biology Undergraduate Student Affairs Office.

● **Academic Integrity**

Academic Integrity is expected of everyone at UC San Diego. This means that you must be honest, fair, responsible, respectful, and trustworthy in all your actions. Lying, cheating, or any other forms of dishonesty will not be tolerated because they undermine learning and the University's ability to certify students' knowledge and abilities. Thus, any attempt to get, or help another get, a grade by cheating, lying or dishonesty will be reported to the Academic Integrity Office and will result in sanctions. Sanctions can include an F in the class and suspension or dismissal from the University. So, think carefully before you act. Before you act, ask yourself the following questions: a: is my action honest, fair, respectful, responsible, and trustworthy, and b) is my action authorized by the instructor? If you are unsure, don't ask a friend, ask your instructor, instructional assistant, or the Academic Integrity Office. You can learn more about academic integrity at academicintegrity.ucsd.edu.

(Source: Bertram Gallant, T. (2017). Teaching for integrity. UC San Diego Academic Integrity Office.)

Refer to:

UCSD Student Conduct Code

(https://students.ucsd.edu/_files/student-conduct/ucsandiego-student-conduct-code_interim-revisions1-16-18.pdf)

Principles of Community
(https://ucsd.edu/about/principles.html)

● **Religious Accommodation**

It is the policy of the university to make reasonable efforts to accommodate students having bona fide religious conflicts with scheduled examinations by providing alternative times or methods to take such examinations. If a student anticipates that a scheduled examination will occur at a time at which his or her religious beliefs prohibit participation in the examination, the student must submit to the instructor a statement describing the nature of the religious conflict and specifying the days and times of conflict.

For final examinations, the statement must be submitted no later than the end of the second week of instruction of the quarter.

For all other examinations, the statement must be submitted to the instructor as soon as possible after a particular examination date is scheduled.

If a conflict with the student's religious beliefs does exist, the instructor will attempt to provide an alternative, equitable examination that does not create undue hardship for the instructor or for the other students in the class.

● Discrimination and harassment

The University of California, in accordance with applicable federal and state laws and university policies, does not discriminate on the basis of race, color, national origin, religion, sex, gender, gender identity, gender expression, pregnancy (including pregnancy, childbirth, and medical conditions related to pregnancy or childbirth), physical or mental disability, medical condition, genetic information, ancestry, marital status, age, sexual orientation, citizenship, or service in the uniformed services (including membership, application for membership, performance of service, application for service, or obligation for service in the uniformed services). The university also prohibits harassment based on these protected categories, including sexual harassment, as well as sexual assault, domestic violence, dating violence, and stalking. The nondiscrimination policy covers admission, access, and treatment in university programs and activities.

If students have questions about student-related nondiscrimination policies or concerns about possible discrimination or harassment, they should contact the Office for the Prevention of Harassment & Discrimination (OPHD) at (858) 534-8298, ophd@ucsd.edu, or reportbias.ucsd.edu.

Campus policies provide for a prompt and effective response to student complaints. This response may include alternative resolution procedures or formal investigation. Students will be informed about complaint resolution options.

A student who chooses not to report may still contact CARE at the Sexual Assault Resource Center for more information, emotional support, individual and group counseling, and/or assistance with obtaining a medical exam. For off-campus support services, a student may contact the Center for Community Solutions. Other confidential resources on campus include Counseling and Psychological Services, Office of the Ombuds, and Student Health Services.

CARE at the Sexual Assault Resource Center

858.534.5793 | sarc@ucsd.edu | https://care.ucsd.edu

Counseling and Psychological Services (CAPS)

858.534.3755 | https://caps.ucsd.edu

Subject to Change Policy

The information contained in this course syllabus, other than the grade and absence policies, may be—under certain circumstances such as mutual agreement to enhance student learning—subject to change with reasonable advance notice.