

# CHEM 36800, Fall 2017

## Biomolecular Structure & Function

### **Instructor:**

Prof. Yujia Xu

Email: [yujia.xu@hunter.cuny.edu](mailto:yujia.xu@hunter.cuny.edu)

Office hours: Friday 11 am – 1 pm *or by appointment*, Room 1304HN

### **Class meeting:**

### **Texts and required readings:**

- Recommended: selected chapters from ‘Physical Chemistry’ by Tinoco/Sauer/Wang/Puglisi/Harbison/Rovnyak
- Recommended: Selected chapters from “The Molecules of Life” by John Kuriyan, Boyana Konforti, and David Wemmer (Garland Science). Individual chapters can be bought on-line (@ \$9/chapter) through the following website: <http://store.vitalsource.com/show/978-1-1350-8892-7>
- Required readings: 1-2 scientific papers will be assigned on a weekly basis.

### **Learning Outcomes:**

After this class, the students are expected to reach the following milestones:

1. Critique peer reviewed journal papers in Biochemistry and related fields.
2. Explain the structural basis of biomacromolecules in function and in self-assembly.
3. Use Protein Data Bank and online tools for structure analysis and viewing.
4. Interpret data of molecular spectroscopy and other methodologies in Structural Biology.
5. Communicate scientific idea through reading, writing, discussion and oral presentation.

### **Course Policies:**

Students are required to conduct themselves in a civil and professional manner so as not to disrupt the learning environment.

**Attendance:** It is mandatory that students attend *all* classes, arrive on time and stay for the entire class. Additionally, students are expected to prepare all assigned reading and discussion points for each class and to be attentive in class. The attendance and the class participation will account for 34% of the final grade (details below).

### **Assignments:**

- 1) Weekly reading reports. In addition to reading assigned papers and leading the discussion on one or more papers, students are required to submit a one page reading report (using the report template) on each assigned paper. The report must be **typed**. No hand written report will be accepted. The hard copy of the report should be handed in at the end of each discussion session. If you do not have access to a printer, you may e-mail me the report *the night before* the class.

- 2) Leading in class discussion: each student will lead one in class presentation (schedule see below).
- 3) Occasional homework assignments.
- 4) A take-home written mid-term exam. The exam will be based on one assigned paper. The exam must be typed, and submitted electronically on the Blackboard within the time period allowed.
- 5) A **final oral/written project**. Students will be directed to choose a research subject related to the course material, select and read in details one or more research articles on the subject, write a short analytical paper based on the reading, and give a 15 min PowerPoint, in-class presentation.

The final written paper should be in range of 2000-2500 words (10-12 pages double-spaced, including figures), should be referenced according to standard practices, should use figures generated by YOU and not copy-pasted from the article, and should follow all guidelines for academic integrity. It should include the following sections: Abstract (<200 words), Introduction, Materials and Methods, Results (including a complete description of the structure, and the methodology used in the research), and Discussion. The Discussion should start with a paragraph of summary of the work. The written assignment must be submitted electronically by **5:00 p.m. on Wednesday, Dec 20**. A late penalty of 10% loss of credit will be assessed for each day the written assignment is submitted late.

### Grading:

Grades for the course will be based upon the following areas:

- 14% on attendance (28 class meetings);
- 20% on participation;
- 28% on reading reports and homework assignments (2pt/repot + homework);
- 10% on take-home exam;
- 28% on final oral and written assignment (equal weight writing and presentation).

Date	Schedule of Topics
1) Mon. Aug 28	INTRODUCTION: Structure of Bio-molecules and the Field of Structural Biology <ul style="list-style-type: none"> <li>• Discussion: DNA replication is semi-conservative, <i>Meselson and Stahl, PNAS (1958) 44:671-682</i>;</li> <li>• Reading assignment (<b>paper #1</b> the classics of structural biology): Watson and Crick, <i>Nature 1953</i>, DNA double helix, please take a look of <b>all 4 papers</b> in the packet available on the Blackboard</li> </ul>
2) Thu. Aug 31	Introduction of the PDB. <b>Bring your computer/tablet!</b>
<b>Mon. 4 Sep</b>	<b>Labor Day, no class</b>
3) Thu. Sep 7	<b>No class (homework: the molecule of the month)</b>
4) Mon. Sep 11	<ul style="list-style-type: none"> <li>• Homework Due.</li> <li>• Discussion of paper #1: how does the knowledge of molecular structure advance our understanding of the biological world</li> </ul>

	<ul style="list-style-type: none"> <li>Coordinator: <u>Amanda Puitiza</u></li> <li>Reading Assignment (<b>paper # 2</b>, Ribosome): Noller et al., Unusual Resistance of Peptidyl Transferase to Protein Extraction Procedures, <i>Science (June 5) 256:1416-1419 (1992)</i></li> </ul>
5) Thu. Sep 14	Lecture, Molecular Spectroscopy: absorbance, CD, fluorescence (Tinoco, Chapter 13)
6) Mon. Sep 18	<ul style="list-style-type: none"> <li>Discussion of Paper #2 by Noller et al: <i>how to formulate a scientific inquiry.</i></li> <li>Discussion coordinator: <u>Abide Ablli-Jah</u></li> <li>Reading Assignment (<b>paper #3</b>, Molecular Spectroscopy): Kardos, J., et al., Phosphorylation as Conformational Switch from the Native to Amyloid State – Trp-Cage as Protein Aggregation Model, <i>J. Phys. Chem. B 2015 119:2946-2955</i></li> </ul>
7) Tue. Sep 19	Lecture, X-ray crystallography I: the crystals and the lattices (Tinoco Chapter 15)
<b>Thu. Sep 21</b>	<b>Hunter closed, no class</b>
8) Mon. Sep 25	<ul style="list-style-type: none"> <li>Discussion of paper #3: the research language of figures, graphs, and Tables.</li> <li>Discussion coordinator: Minhua Chen</li> <li>Reading Assignment (<b>paper #4</b>, Protein Crystallography): Xu, W., et al., ‘Crystal Structure of c-Src Reveal Features of Its Autoinhibitory Mechanism’, <i>Mol. Cell 3:629-638, May 1999</i></li> </ul>
9) Thu. Sep 28	Lecture, X-ray crystallography II: x-ray diffraction (Tinoco Chapter 15)
10) Mon. Oct 2	<ul style="list-style-type: none"> <li>Discussion of paper #4: the structure by X-crystallography</li> <li>Discussion coordinator: <u>Maisha Damus</u></li> <li><del>Reading assignment: take home exam</del></li> </ul>
11) Thu. Oct 5	Lecture Principles of protein-nucleic acid recognition (Kuriyan, Part IV) <i>Reading assignment: take home exam</i>
<b>Mon 9 Oct.</b>	<b>Columbus Day, no class</b>
12) Thu. Oct 12	<b>COMPUTER LAB II (Lab F, Hunter computer center): introduction to spdbv</b> <ul style="list-style-type: none"> <li><b>Take home due</b></li> <li>Reading assignment (<b>paper #5</b>, Cascade type I): Nuñez, J., et al., Cas-1-Cas2 Complex Formation Mediates Spacer Acquisition during CRISPR-Cas Adaptive Immunity, <i>Nat. Struc. Mol. Biol, 21(6): 528-534 (June, 2014)</i></li> </ul>
13) Mon 16 Oct	Lecture, the CRISPR-Cas adaptive immune system
14) Thu. Oct 19	<ul style="list-style-type: none"> <li>Discussion of paper #5: Cascade and the adaptive immunity</li> <li>Discussion coordinator: <u>Muhammad Farooq</u></li> <li>Reading assignment (<b>paper #6</b>, Type III CRISPR-Cas): Spilman, M., et al., Structure of an RNA Silencing Complex of the CRISPR-Cas Immune System, <i>Mol. Cell 52:146-152, (10) Oct, 2013</i></li> </ul>
15) Mon. Oct 23	Lecture, Light/electron scattering and Electron microscopy
16) Thu. Oct 26	<ul style="list-style-type: none"> <li>Discussion of paper # 6: structure of large complexes by Cryo-EM</li> <li>Discussion coordinator: <u>Carl Guenst</u></li> </ul>

	<ul style="list-style-type: none"> <li>• Reading assignment (<b>paper #7</b> type II Cas9): Anders, C., et al., Structure Basis of PAM-dependent Target DNA Recognition by the Cas9 Endonuclease <i>Nature</i> 513:569-573 (25 Sep, 2014)</li> </ul>
17) Mon. Oct 30	Lecture, Protein NMR spectroscopy (Tinoco, Chapter 14)
18) Thu. Nov 2	<ul style="list-style-type: none"> <li>• Discussion of paper #7: the type II Cas9 and gene editing</li> <li>• Discussion coordinator: <u>Julia Korobenko</u></li> <li>• Reading Assignment (<b>paper #8</b>, NMR): Harper et al., Structural Basis of a Phototropin Light Switch <i>Science</i>, 302:1541-1544 (12 Sep, 2003)</li> </ul>
19) Mon. Nov 6	Lecture: XFEL the new tools of structural biology
20) Thu. Nov 9	<ul style="list-style-type: none"> <li>• Discussion of paper #8: catch the conformational changes in action</li> <li>• Discussion Coordinator: <u>James McGowan</u></li> <li>• Reading Assignment (<b>paper #9</b>, the Riboswitch): Stagno, J. R., et al., Structures of riboswitch RNA reaction states by mix-and-inject XFEL serial crystallography, <i>Nature</i>, 541:242-246, 12 Jan. 2017</li> </ul>
21) Mon. Nov 13	The activation potential of neurons (Kuriyan Chapter 11)
22) Thu. Nov 16	<ul style="list-style-type: none"> <li>• Discussion of paper #9: the newest in structural biology.</li> <li>• Discussion Coordinator: <u>Dominick Harrison</u></li> <li>• Reading assignment (<b>paper #10</b>, K<sup>+</sup> channel): Doyle, D., et al., The Structure of the Potassium Channel: Molecular Basis of K<sup>+</sup> Conduction and Selectivity, <i>Science</i> 280:69-77, 3 April, 1998</li> </ul>
23) Mon. Nov 20	<ul style="list-style-type: none"> <li>• Discussion of paper #10: ion selectivity of K<sup>+</sup> channel</li> <li>• Discussion coordinator(s): <u>Orak Oleksander</u></li> <li>• Reading assignment (<b>paper 11</b>, Voltage gating): Jiang, Q-X., Electron microscopy analysis of KvAP Voltage-Dependent K<sup>+</sup> Channels in an Open Conformation <i>Nature</i> 430:806-810 (12 Aug., 2004)</li> </ul>
<b>Thus. 23</b>	<b>Thanksgiving</b>
24) Mon. Nov 27	<ul style="list-style-type: none"> <li>• Discussion of paper #11: the structural basis of voltage gating</li> <li>• Discussion coordinator: <u>Vanita Parmar</u></li> <li>• Reading Assignment (<b>paper 12</b>, Protein Design): Fleishman et al, Computational Design of Proteins Targeting the Conserved Step Region of Influenza Hemagglutinin, <i>Science</i> 332:816-821 (13 May, 2011)</li> </ul>
25) Thu. Nov 30	<ul style="list-style-type: none"> <li>• Discussion of paper #12: a better design than nature?</li> <li>• Discussion coordinator: Faith Titilawo</li> </ul>
26) Mon. Dec 4	Presentations (15 min including questions, training and critique): Amanda Puitiza, Abide Balli-Jah, <del>Minhua Chen</del> , and Maisha Damus
27) Thu. Dec 7	Presentations (15 min, critique): Muhammad Farroq, Carl Guerst, Julia Korobenko, and James McGowan
28) Mon. Dec 11	Presentations (15 min, critique): Orak Oleksandr, Vanita Parmar, Faith Titilawo, and Gurpreet Kaur
Dec 14-21	<b>Final Paper due 20 Dec. 5 pm</b>

**Policy on academic integrity:** Students must assume responsibility for maintaining honesty in all work submitted for credit. Violations to academic integrity include cheating, plagiarism, fabrication, purchasing the work of others and submitting it as one's own, allowing one's work to be used by others, multiple submission of work, and misuse of computers. To avoid plagiarism, it is necessary to give credit whenever you using another person's idea, opinion, or theory; any data, facts, statistics, graphs, drawings that are not common knowledge; quotations of another person's actual spoken or written words; a paraphrase of another person's spoken or written words. *STATED SUCCINCTLY, COPYING EVEN ONE SENTENCE OF WORK BY ANOTHER, OR "BORROWING" SOMEONE ELSE'S DATA OR IDEA, WHETHER PUBLISHED OR UNPUBLISHED, WITHOUT EXPLICITLY CITING THE SOURCE, IS PLAGIARISM, and will be dealt with severely.* Violations of academic integrity will be addressed in accordance with The City University of New York policy on academic integrity.

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### Hunter College required statements for syllabi

1. Academic Integrity Statement: "Hunter College regards acts of academic dishonesty (e.g., plagiarism, cheating on examinations, obtaining unfair advantage, and falsification of records and official documents) as serious offenses against the values of intellectual honesty. The College is committed to enforcing the CUNY Policy on Academic Integrity and will pursue cases of academic dishonesty according to the Hunter College Academic Integrity Procedures."
2. ADA Statement: "In compliance with the ADA and with Section 504 of the Rehabilitation Act, Hunter College is committed to ensuring educational access and accommodations for all its registered students. Hunter College's students with disabilities and medical conditions are encouraged to register with the Office of AccessABILITY for assistance and accommodation. For information and appointment contact the Office of AccessABILITY located in Room E1214 or call (212) 772-4857 /or VRS (646) 755-3129."
3. Hunter College Policy on Sexual Misconduct "In compliance with the CUNY Policy on Sexual Misconduct, Hunter College reaffirms the prohibition of any sexual misconduct, which includes sexual violence, sexual harassment, and gender-based harassment retaliation against students, employees, or visitors, as well as certain intimate relationships. Students who have experienced any form of sexual violence on or off campus (including CUNY-sponsored trips and events) are entitled to the rights outlined in the Bill of Rights for Hunter College.
  - a. Sexual Violence: Students are strongly encouraged to immediately report the incident by calling 911, contacting NYPD Special Victims Division Hotline (646-610-7272) or their local police precinct, or contacting the College's Public Safety Office (212-772-4444).
  - b. All Other Forms of Sexual Misconduct: Students are also encouraged to contact the College's Title IX Campus Coordinator, Dean John Rose (jtrose@hunter.cuny.edu or 212-650-3262) or Colleen Barry (colleen.barry@hunter.cuny.edu or 212-772-4534) and seek complimentary services through the Counseling and Wellness Services Office, Hunter East 1123.

CUNY Policy on Sexual Misconduct Link:

<http://www.cuny.edu/about/administration/offices/1a/Policy-on-Sexual-Misconduct-12-1-14-with-links.pdf>"