CHEM 33300/CHEM63300: Computational Drug Discovery

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Course Webpage: Hunter Blackboard

Time & Location:
Lecture
Office hour

Pre-requisites: CHEM 376 or BIOL 300 or permission of instructor.

About this course:

- This is an advanced course designed for upper-level undergraduate and graduate students. The main goal of this course is to teach you how to acquire new knowledge from primary literature. This is important because the newest topics in science are not in the textbooks; they are in primary scientific literature.
- In each module, you will first learn basic concepts through lectures and web exercises. Then, you will analyze primary literature. The four modules covered in CHEM33300/63300 are:
  - Drug-macromolecule interactions
    - Structure-based drug design
  - Virtual screening
    - Docking
  - Microbial natural products/Metabolic engineering
    - Discovery of drug leads from microorganisms
  - Personalized medicine
    - Discovery of biomarkers for drug sensitivity, resistance, and safety
- **Learning Objectives (LO):** Provided at the end of this syllabus.
- Students will be **required** to be fully prepared for each lecture (by completing homework assignments). Unprepared students will be asked to leave the class.
- Students will be **required** to actively participate in discussions during the class.

Textbook: Reading materials will be provided by the instructor.

Grading: Homework assignments – six essays (1 page each) (90 pts), Participation in in-class discussions (30 pts), Amino acid quiz (20 pts), Final presentation & report (160 pts). **Grade range (CHEM333, approximate):** A (270-300 pts), B (240-269 pts), C (210-239 pts), D (180-209 pts), F (below 179 pts). No CR/NC grade in this course. **Grade range (CHEM633, approximate):** A (270-300 pts), B (240-269 pts), C (210-239 pts), F (below 209 pts).

Final presentation & report (CHEM333): Students in CHEM33300 will be required to give an oral presentation and submit a written report on a research article related to the topics covered in this class. This requirement will test the ability of students to critically analyze primary scientific literature.

Final presentation & report (CHEM633): Students in CHEM63300 will be required to give an oral presentation and submit a written report on a research article related to the topics covered in this class. *In addition, students will be required to propose a new study based on the article.* The first requirement will test the ability of students to critically analyze primary literature. The second requirement will test the ability of students to formulate a new testable hypothesis, and propose approaches to test the hypothesis.

Academic dishonesty: If any form of academic dishonesty is found, involved student(s) will be automatically given F with a note stating "Failed, due to academic dishonesty" on their transcripts. Student(s) will also be subjected to disciplinary actions according to the school guideline.

Policy on Incomplete Grade: Incomplete (IN) grade would be considered if a student maintained a passing grade (from class-participation, essays, and quiz), but cannot complete the course because of unavoidable reasons, e.g., a medical or personal emergency. Documented proof will be required for the consideration of IN grade.

"In compliance with the **American Disability Act of 1990 (ADA) and with Section 504 of the Rehabilitation Act of 1973**, Hunter College is committed to ensuring educational parity and accommodations for all students with documented disabilities and/or medical conditions. It is recommended that all students with documented disabilities (Emotional, Medical, Physical and/ or Learning) consult the Office of AccessABILITY located in Room E1124 to secure necessary academic accommodations. For further information and assistance please call (212- 772- 4857)/TTY (212- 650- 3230)."

Class & Exam Schedule:

Date		Topic
Monday	29-Jan-18	***Introduction***
Thursday	1-Feb-18	***Module 1:*** Drug-macromolecule interactions (Lecture)
Monday	5-Feb-18	***Module 1:*** Drug-macromolecule interactions (Lecture)
Thursday	8-Feb-18	***Module 1:*** Drug-macromolecule interactions (Web exercise)
Monday	12-Feb-18	No Class – Lincoln's Birthday – College is closed.
Thursday	15-Feb-18	***Module 1:*** **Drug-macromolecule interactions (Literature trial 1****) – Short essay due
Monday	19-Feb-18	No Class – Presidents' Day – College is closed.
Tuesday*	20-Feb-18	***Module 1:*** Drug-macromolecule interactions (Web exercise)
Thursday	22-Feb-18	***Module 1:*** Drug-macromolecule interactions (Literature trial 2) – Short essay due
Monday	26-Feb-18	***Module 2:*** Virtual screening (Lecture)
Thursday	1-Mar-18	***Module 2:*** Virtual screening (Lecture) –**Quiz on Amino Acids**
Monday	5-Mar-18	***Module 2:*** Virtual screening (Web exercise)
Thursday	8-Mar-18	***Module 2:*** Virtual screening (Literature trial 3) – Short essay due
Monday	12-Mar-18	***Module 2:*** Virtual screening (Web exercise)
Thursday	15-Mar-18	***Module 2:*** Virtual screening (Literature trial 4) – Short essay due
Monday	19-Mar-18	***Module 3:*** Metabolic engineering (Lecture)
Thursday	22-Mar-18	***Module 3:*** Metabolic engineering (Lecture)
Monday	26-Mar-18	***Module 3:*** Metabolic engineering (Web exercise)
Thursday	29-Mar-18	***Module 3:*** Metabolic engineering (Literature trial 5) – Short essay due
Monday	2-Apr-18	No Class – Spring Recess
Thursday	5-Apr-18	No Class – Spring Recess
Monday	9-Apr-18	***Module 3:*** Metabolic engineering (Web exercise)
Thursday	12-Apr-18	***Module 3:*** Metabolic engineering (Literature trial 6) – Short essay due
Monday	16-Apr-18	***Module 4:*** Personalized medicine (Lecture)
Thursday	19-Apr-18	***Module 4:*** Personalized medicine (Lecture/Web exercise)
Monday	23-Apr-18	***Module 4:*** Personalized medicine (Literature trial 7) – Short essay due
Thursday	26-Apr-18	***Module 4:*** Personalized medicine (Web exercise)
Monday	30-Apr-18	***Module 4:*** Personalized medicine (Literature trial 8) – Short essay due
Thursday	3-May-18	Final presentations 1 (4-5 students)
Monday	7-May-18	Final presentations 2 (4-5 students)
Thursday	10-May-18	Final presentations 3 (4-5 students)
Monday	14-May-18	Final presentations 4 (4-5 students)
Monday	21-May-18	Final Report due

*Classes follow a Monday schedule

**Practice session.

Note: There will be eight literature trials. The first trial will be a practice session; your participation and essay for the first trial will not be graded. Literature trials 2-8 will be graded (participation and essay). The trial with the lowest grade will be dropped. If a student is absent in one of the trials, the missed trial will be automatically dropped. *There will be no make-up opportunities for missed literature trials.*

CHEM33300/CHEM63300 Computational Drug Discovery
Learning Objectives

	Key LO	Assignments	Assessment	Analysis	Expected Outcome
1	Able to understand primary literature on computational drug discovery	Homework assignments.	Short essays	Students will be able to understand the following aspects of primary literature: (1) the knowledge gap and its importance; (2) approaches to fill the gap;	For mastery students are expected to earn at least 70% of the points available for this LO.
2	Able to formulate critiques on primary literature	Homework assignments. Literature discussions. Final presentation (critiques)	Short essays. Participation in literature discussions. Critiques (Final presentations)	Students will be able to evaluate the following aspects of primary literature: (1) significance; (2) approach; (3) presentations.	For mastery students are expected to earn at least 70% of the points available for this LO.
3	Able to defend his/her scientific conclusions on primary literature	Literature discussions. Final presentation and report.	Literature discussions. Final Presentation & Report.	Students will be able to defend his/her own evaluations.	For mastery students are expected to earn at least 70% of the points available for this LO.
4	**(CHEM633 only)** Able to generate and defend an original hypothesis.	Final presentation and report (original research proposal)	Final presentation and report (original research proposal)	Students will be able to generate and defend a hypothesis.	For mastery students are expected to earn at least 70% of the points available for this LO.

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/la/Policy-on-Sexual-Misconduct-12-1-14-with-links.pdf"