

Chem 38857 - Medicinal Chemistry

Instructor: Wayne Harding

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Lecture Times:

Location:

Office Hours:

Brief Course Description: The course will cover principles of drug design, drug discovery and drug action.

Learning Outcomes:

After completing this course students should be able to:

1. Explain the drug discovery process from hit-to-lead generation to drug approval.
2. Recognize functional groups within a drug and discuss how the specific features of a given functional group contribute to the overall properties of the drug, including: solubility, acid/base properties, ADMET, and ligand-binding site interactions.
3. Describe tools and experimental methods used to discover and develop new drugs.
4. Describe the metabolic fate of functional groups and how metabolic changes to a drug affect physical, pharmacodynamic, and pharmacokinetic properties.
5. Explain the mechanistic principles underlying the therapeutic actions of selected drugs
6. Apply the above topics to real-world drug development situations.

Pre-requisites: Chem. 37600 (Biochemistry 1)

Number of credits: 3

Recommended Textbook: An Introduction to Medicinal Chemistry, by Graham Patrick, 5th edition, ISBN-13: 978-0199697397.

Other Reading Materials: Notes and handouts will be provided in class and on Blackboard.

Exams/Grading: There are a total of **400** points for the course constituted as follows.

<u>Exam 1:</u>	100 points
<u>Exam 2:</u>	100 points
<u>Exam 3:</u>	100 points
<u>Presentations:</u>	70 points
<u>MCQs for presentation :</u>	5 points
<u>Class participation:</u>	25 points

Exams: All exams are **mandatory**. If you miss an exam, you must present verifiable proof of the reason for missing the exam within 24 hours. Otherwise, there will be **NO** make-up exam. Make-up exams are generally much **harder**.

Presentations: Students will be grouped (two persons per group) and each group will give a presentation on a drug. Presentations should be done using Powerpoint and should last no longer than 25 minutes. There will be additional time for questions at the end of the presentation. A second group will be selected to lead a discussion (lasting approx. 5 min) after each presentation. Powerpoint presentation files should be emailed to the instructor at least one week prior to the actual presentation for distribution to the class.

Below is the list of drugs (trade names) to be used for presentation topics:

1. Prozac
2. Gleevec
3. Abilify
4. Aricept
5. Sustiva
6. Nexium
7. Crestor
8. Lyrica
9. Lipitor
10. Cymbalta
11. Plavix
12. Januvia
13. Invokana
14. Flomax
15. Belsomra
16. Tamiflu

The following information will be useful to include in your presentation.

(Although this list is meant to provide guidance, it is not an exhaustive)

- How was the drug discovered – natural source, high throughput screen, serendipity?
- Describe methods for synthesis of the drug
- What is the biological target of the drug?
- Describe in detail the normal and abnormal function (diseased state) of the biological target
- Describe in detail how the drug functions. Provide specific information on receptor-ligand interactions and other details on the mechanism of action of the drug.
- What is known about the structure-activity relationships of the drug at the biological target?
- What is the current market for the drug?
- What are current, past, predicted sales of the drug?
- What other drugs are competing for the same market?
- Discuss toxicity, side effects, drug interactions and pharmacokinetics of the drug
- Provide your own view on what remains to be done in the (disease) area. What significant challenges remain to be overcome to achieve optimal treatment and how do you envisage that this may be achieved?
- Any other information that you consider significant or interesting

MCQ's for presentation: Students should prepare 5 multiple choice questions (and indicate answers) based on their presentation. The MCQs should be emailed to the instructor prior to the presentation.

Class Participation: Students will receive points for participating in class discussions and during presentations by peers.

Projected grade cut-offs: A, B, C grades are further divided into +/- subgrades according to Hunter guidelines.

- A. 360 - 400 points
- B. 320 - 359 points
- C. 280 – 319 points
- D. 240 – 279 points
- F. 0 - 239 points

Policy on Incomplete grade: Incomplete (IN) grade may be given if a student has a reasonable chance of passing the course but cannot complete it because of a valid reason. In order to be considered for the IN grade, students need to present verifiable proof. For further information on grading guidelines, see the Hunter College Catalog or visit <http://md2.hunter.cuny.edu/webgrade/regmemo.jsp> for College grading policy on CR/NC, INC, WU etc. These guidelines will be followed for the course.

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>”

Tentative Course Schedule

Date	Topic
	MODULE 1 – Drug targets and interactions
Jan 30	Course Introduction/Drug Discovery Process
Feb. 2	Functional groups and molecular properties
Feb. 6	Receptors as drug targets I
Feb. 9	Receptors as drug targets II
Feb. 13	<i>No class – Lincoln's Birthday</i>
Feb. 15	Receptors as drug targets III (Wed; class follows Mon schedule)
Feb. 16	Enzymes as drug targets
Feb. 20	<i>No class- President's Day</i>
Feb 23	EXAM 1
Feb. 27	MODULE 2 – Drug discovery and
Mar. 2	Target and lead identification
Mar. 6	ADME I
Mar. 9	ADME II
Mar. 13	Drug design I
Mar. 16	Drug design II
Mar. 20	Drug design III
Mar. 23	EXAM 2
	MODULE 3 – Medicinal chemistry of selected drug classes
Mar. 27	Antibacterials I
Mar. 30	Antibacterials II
Apr. 3	Cholinergics/Anticholinergics I
Apr. 6	Cholinergics/Anticholinergics II
Apr. 10	<i>No class- Spring Break</i>
Apr. 13	<i>No class- Spring Break</i>
Apr. 17	<i>No class- Spring Break</i>
Apr. 20	Antiulcer agents (Monday Schedule)
Apr. 24	Opioid analgesics
April 27	EXAM 3
May 1	Presentations (Groups 1 and 2)
May 4	Presentations (Groups 3 and 4)
May 8	Presentations (Groups 5 and 6)
May 11	Presentations (Groups 7 and 8)
May 15	Presentations (Groups 9 and 10)