

Foundations in Drug Discovery
16:663:501:01; 30:715:451:01
3 credits
Fall – 2025

Course Coordinator(s):

Matthew Moschitto, Assistant Professor. Department of Medicinal Chemistry William Levine Hall, Room 330; m.moschitto@rutgers.edu; Office Hours: by appointment only

Course Faculty: (include all faculty and guest lecturers)

Jun Wang; Ernest Mario School of Pharmacy, Professor, *Department of Medicinal Chemistry, William Levine Hall, Room 326; junwang@pharmacy.rutgers.edu. Office Hours: TBD, by appointment.*

Course Description: Foundations in Drug Discovery covers the important biochemical processes involved in the development of pharmaceuticals. This course provides an overview of the drug discovery process and provides a foundation for students interested in a career in drug discovery by applying both organic and biochemical principles. There are three parts to this course: (i) Understanding the drug discovery process (2) Common targets in drug discovery including receptors, kinases, GPCRs, ion channels, metabolic enzymes, and DNA; and (3) inhibitor design and evaluation including assay development, enzymology, PK/PD studies, and metabolism. This course is designed as an introductory graduate course or an advanced undergraduate course for students who have taken two semesters of organic chemistry.

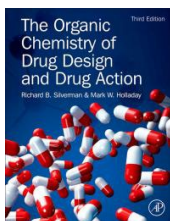
Course Meeting Time(s) and Location(s):

Tuesday: 11:00 AM – 12:20 PM
Friday: 1:00 PM – 2:20 PM
EMSOP Room 249

Course Materials

Required and Recommended Texts:

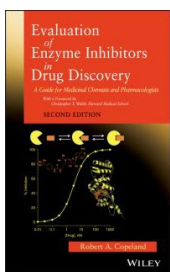
The course generally follows two textbooks. The reading assigned are not required but are suggestions to supplement the lecture material. These textbooks are not required for purchase but are incredibly useful textbooks for any Medicinal Chemist. Handouts will be posted on the class canvas page and similarly are suggestions (unless otherwise noted in a problem set).



1. Silverman RB, Holladay MW. *The Organic Chemistry of Drug Design and Drug Action*. Third edition. Amsterdam: Elsevier; 2014.

This book is available online free from Rutgers Library at:

<https://ebookcentral.proquest.com/lib/rutgers-ebooks/detail.action?docID=5754489>



2. Copeland, R. A. *Evaluation of enzyme inhibitors in drug discovery: A guide for medicinal chemists and pharmacologists*. Somerset: John Wiley & Sons, Incorporated, 2013.

This book is available online free from Rutgers Library at:

<https://ebookcentral.proquest.com/lib/rutgers-ebooks/detail.action?docID=1120975#>

Computer Software: This course will require the use of various software platforms. This software is available free of charge from the university and can be downloaded at software.rutgers.edu unless otherwise noted. If you need assistance, please ask. A computer lab is located in EMSOP room 323. Please email Mary Li (shikeli@pharmacy.rutgers.edu) if you require access. The following software will be used or discussed in class:

1. Chemdraw
2. Endnote
3. Origin Pro
4. Pymol (<https://pymol.org/2/>)

Method of Instruction:

- Lectures will be given in person only.
- All lecture material including notes, powerpoint slides, problems, etc. will be posted on Canvas.

Class Schedule:

Date	Lecture Number	Topic	Specific topics	Readings	Instructor	PS due date
09/02	1	Introduction to Drug Discovery		Silverman 1	JW1	
09/05	2	Introduction to drug discovery		Silverman 2	JW2	
09/09	3	Organic Principles in Drug Discovery	Bonding, Stereochemistry, pKa	Silverman 3.1-3.22	MJM1	
09/12	4	Drug Receptor Interactions	H-Bonds, covalent bonding, electrostatic, hydrophobic interactions	Silverman 3.23-3.3	MJM2	
09/16	5	Enzyme Catalysis	Enzymatic catalysis, cofactors	Silverman 4; 5.1	MJM3	
09/19	6	Mechanism Based enzyme inactivators		Silverman 5.3	MJM4	PS1
09/23	7	Targeting Proteases		Lecture slides	JW3	
09/26	8	Targeting Kinases		Lecture slides	JW4	
09/30	10	Targeting GPCRs		Lecture slides	JW5	
10/03	11	Targeting Ion Channels		Lecture slides	JW6	
10/07	E1	EXAM 1	Lectures 1-10			
10/10	O	No Class	Attend PACSFOCS			
10/14	12	Targeting DNA		Silverman 6	MJM5	
10/17	13	Targeting DNA			MJM6	
10/21	14	Inhibitor Evaluation	Enzyme kinetics Reversible and Irreversible inhibitors	Copeland 2.4-2.6, 3.1-3.6, 5.1-5.4,	MJM7	
10/24	15	Inhibitor evaluation	Slow binding inhibitors Tight binding inhibitors	Copeland 6.1-6.4, 9.1-9.2	MJM8	PS2 (Targets)
10/28	16	Inhibitor Evaluation			MJM9	

10/31	17	Assays	Assay set up; fluorescence, ITC, DSF,	Copeland 4	MJM10	
11/04	18	Assays		Copeland 4	MJM11	
11/07	O	Open			MJM	PS3 (Eval)
11/11	E2	Exam 2	Lectures 11-18			
11/14	19	Drug Resistance and synergism		Silverman 7	MJM12	
11/18	20	Antimicrobial drug resistance			JW7	
11/21	21	Drug Metabolism	CH/N/O oxidations Reductions	Silverman 8	MJM13	
11/26 (WED)	22	Drug Metabolism	Phase II transformations		MJM14	
12/02	23	<i>In vitro</i> pharmacokinetics in drug discovery		Copeland 10	JW8	
12/05	24	<i>In vivo</i> pharmacokinetics in drug discovery			JW9	
12/09	O	Projects/Open			MJM15	PS4
	FINAL		Lectures: 50%: 19-24 50% 1-18			

Changes in lecture scheduling may need to be made at the discretion of the course coordinator. Please see canvas for updated course schedule

Attendance and Participation Policy

Students are expected to attend all lectures; if you expect to miss one or more lectures, please use the University absence reporting website <https://sims.rutgers.edu/ssra/> to indicate the date and reason for your absence. An email is automatically sent to the faculty coordinator. If you will need to miss an exam, please contact Dr. Moschitto (m.moschitto@rutgers.edu)

Assessment and Grading:

- Two midterm exams and a final will be given. Each midterm exam will be 3 h in length and be composed of the preceding sections' material. The final will be split between material from the first two exams and new material. Exam material will be based on lecture and problem set material only.
- Four problem sets/projects will be assigned in this course. Problem sets will be posted on Canvas. Their due date will be listed on canvas and in the syllabus. Students should not share answers with each other and work independently. Copying another student's answers will be considered plagiarism (see below). It is permitted, however, to discuss the problems between students. It is in your best interest to work through the problems

individually to understand the material. Students should not google or look up and copy answers from online sources either, this includes programs such as Reaxys and Scifinder.

	<i>Percent Grade</i>
<i>Problem Sets</i>	<i>20</i>
<i>Exam 1</i>	<i>25</i>
<i>Exam 2</i>	<i>25</i>
<i>Final Exam</i>	<i>25</i>
<i>Class Participation</i>	<i>5</i>

Grading Scale:

The following grading scale can be used as a guide; however, course grades can change depending on overall course average.

A = 90-100 (4.0)
 B+ = 80-89 (3.5)
 B = 70-79 (3.0)
 C+ = 60-69 (2.5)*
 C = 50-59 (2.0)*
 F = <50 (0.0)

*Contingent on completing all problem sets and exams, as well as maintaining satisfactory attendance and participation in class. Otherwise, a D/F may be awarded.

In the event of course failure for PharmD students: *After a student receives an F as the final grade for this course, the sole remediation option is to repeat the course when next offered, subject to approval of the School's Scholastic Standing Committee.*

Accessibility:

Rutgers University is committed to the creation of an inclusive and safe learning environment for all students and welcomes students with disabilities into all the University's educational programs. The Office of Disability Services (ODS) is responsible for the determination of appropriate accommodations for students.

Once a student has completed the ODS process (registration, initial appointment, and submitted documentation) and reasonable accommodations are determined a Letter of Accommodation (LOA) can be requested and will be sent to the student and instructor. This should be done as early in the semester as possible as accommodations are not retroactive, and a discussion should occur about how the accommodations will be implemented.

More information can be found at <https://ods.rutgers.edu/>.

To begin this process, please complete the [registration form](https://webapps.rutgers.edu/student-ods/forms/registration) (<https://webapps.rutgers.edu/student-ods/forms/registration>).

You can contact ODS at 848-202-3111 or via email at dsoffice@echo.rutgers.edu for any questions.

Academic Integrity Policy:

Students are subject to the University academic integrity policy, which is provided to new students at orientation and is also available online from

<https://academicintegrity.rutgers.edu> at:

<https://academicintegrity.rutgers.edu/sites/default/files/pdfs/current.pdf>

This policy was updated in the summer of 2020.

For PharmD students: the School of Pharmacy has also established an ad hoc committee on academic integrity. The committee has membership from both the faculty and student body. Given the serious nature of the work health care workers provide, academic integrity and honesty are of the utmost importance in pharmacy school. The faculty of the Ernest Mario School of Pharmacy approved the following statements for both students and faculty which were developed by the committee in conjunction with student leadership.

For Graduate Students: Please see the Department of Medicinal Chemistry Graduate Handbook for Academic Integrity statements.

In the new policy, violations of academic integrity are generally divided into three categories: Level 1, Level 2, and Level 3.

- Level 1 violations may occur as a result of inexperience or lack of malicious intent by the person committing the violation.
- Level 2 violations include misconduct of a more serious character or misconduct that affects a major, significant, or essential portion of work done to meet course requirements. These violations demonstrate premeditation or may have posed harm to others. The student alleged to have committed the violation may have one or more previous violations.
- Level 3 violations represent the most serious breaches of conduct. They may involve a serious violation of a professional code of conduct; may include extreme cases of dishonesty and maliciousness or violations of law; and/or are likely to cause direct harm to others.

The procedures for adjudicating alleged violations of academic integrity are different for Level 1, Level 2, and Level 3 violations. Students are referred to the full policy at the link above for examples of violations and potential sanctions. When a student is accused of one or more Level 3 violations that include alleged violations of law or a professional code of conduct, or when it is reasonable to believe that the student is likely to cause direct

harm to others, they may be removed from a course, clinical, or internship setting on an interim basis, with the approval of the dean of the school.

The following are some general examples of the responsibilities of students:

- To understand the definition of scholastic dishonesty.
- To understand the instructions for each assignment, quiz, or examination.
- To refrain from committing any acts of scholastic dishonesty.
- To take appropriate action when acts of scholastic dishonesty are observed.
- To understand the importance of confidentiality in pharmacy practice and the ramifications of breaching patient trust.
- To engage in appropriate classroom and laboratory conduct.

As noted, this list serves only as an example. The entire Academic Integrity Policy should be reviewed, downloaded and printed from the link above. It is the student's responsibility to review the entire policy for more specific information regarding specific infractions and penalties. Violations of any of these principles will result in prosecution by Ernest Mario School of Pharmacy, the Department of Medicinal Chemistry, the Graduate School, and/or the Student Judicial Affairs department. Severe penalties may be levied which may include expulsion from Ernest Mario School of Pharmacy as well as from the entire Rutgers University.

Class recordings:

Audio and video recordings are not allowed.

PharmD Program-Level Educational Outcomes and Course Learning Objectives:

Program Level Educational Outcomes

2025 ACPE Standard 2 : Curricular Outcomes (CO)

Domain	Sub-Domain # Name	One Word Descriptor	Outcome Description	*Bloom's Taxonomy Level
Knowledge	2.1.a Scientific thinking	Learner	The graduate is able to seek, analyze, integrate, and apply foundational knowledge of medications and pharmacy practice (biomedical; pharmaceutical; social, behavioral, and administrative; and clinical sciences; drug classes; and digital health).	Level 1 Level 2
Skills	2.1.b Problem solving process	Problem-Solver	The graduate is able to use problem solving and critical thinking skills, along with an innovative mindset, to address challenges and to promote positive change.	Level 1 Level 2

2025 ACPE Appendix I Categories:

ACPE Appendix 1 Categories	*Bloom's Taxonomy Levels
Medicinal Chemistry	Level 1, Level 2

Course Learning Objectives

At the conclusion of this course learners will be able to:

1. Understand fundamental concepts in medicinal chemistry and drug discovery
2. Attain the ability to apply concepts in drug discovery research

Assessment Mapping Table

Assessment	Mapping COs	ACPE Appendix 1	*Bloom's Levels
<i>Exam 1</i>	<i>2.1a, 2.1b</i>	<i>Medicinal Chemistry</i>	<i>1,2</i>
<i>Exam 2</i>	<i>2.1a, 2.1b</i>	<i>Medicinal Chemistry</i>	<i>1,2</i>
<i>Final Exam</i>	<i>2.1a, 2.1b</i>	<i>Medicinal Chemistry</i>	<i>1,2</i>
<i>Problem Sets</i>	<i>2.1a, 2.1b</i>	<i>Medicinal Chemistry</i>	<i>1,2</i>