

CHEM 6420/4420
Drug Discovery: Theory and Practice
Spring 2019

Instructor:

Dr. Ming Luo

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Phone: 404-413-6608

Lecture Schedule & Room:

Tuesday and Thursday 5:30-8:15 pm;

Landale 620

Office Hours:

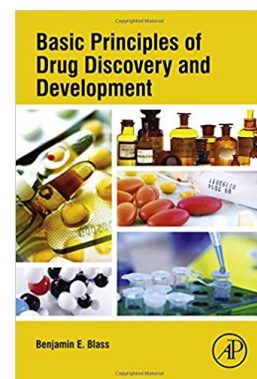
4:00pm-5:00pm, NSC 585, Tuesday and Thursday. Appointment by email.

Office hours are suspended on the day of the exams, and no questions will be answered on the day of the exams.

Students desiring to discuss more in-depth about a topic or career plans may schedule an appointment via email.

Textbook:

Basic Principles of Drug Discovery and Development, 1th edition, by Benjamin Blass (ISBN-13: 978-0124115088, Academic Press) is a good reference, but not required.



Software:

Use PyMol for structure display, compound design and overlay

(<https://pymol.org/edu/?q=educational/>)

After positioning your design in the active site, calculate the score.

Use (<http://pasilla.health.unm.edu/tomcat/biocomp/convert>) to convert a ligand.pdb file to a ligand.mol2 file.

Use DSX^{ONLINE} (<http://pc1664.pharmazie.uni-marburg.de/drugscore/index.php>) to calculate the score.

PDB files will be provided via iCollege.

Course Objective:

A comprehensive and integrated review of modern techniques used in drug discovery. Students will carry out a hand-on exercise and write a report. There is a total of 12 in-class lectures.

Expected Learning Outcomes:

1. Understand the essential processes and principles for selecting the drug target.
2. Understand the principles for selecting drug candidates.
3. Learn how to apply a number of tools to identify drug candidates.

For graduate level students, they would be able to apply the principles and tools in one of their own research project or an example project assigned in the course.

Tests and Assignments:

10 pop quizzes of 10 points per quiz,	= 100 (10x10)
Two in-class Mid-term exams of 100 points each,	
Mid-terms	= 200
Student report	= 100
One comprehensive final exam	= 200
Total	= 600

Exams schedule (Please mark your calendar):

April 2 (T) in class exam 1

April 18 (T) in class exam 2/student report

April 23 (Th) final exam

No make-ups or rescheduling of exams will be carried out under any circumstance

The final grade will be counted against the possible points out of 600 (10 quizzes + 2 in class exams + student report + final exam). The final exam is mandatory, and it must be taken on April 23. You are responsible for withdrawing before the deadline if you need to do so. If in-class exams are missed for legitimate reasons, you should seek a hardship withdrawal or an incomplete. If you do not withdraw and miss the final exam, or more than two in-class exams, then zeros will be assigned for your grades.

Projected Grading Scale (≥):

A+: 95%, A: 90%; A-: 86%; B+: 80%; B: 75%; B-: 70%; C+: 66%; C: 63%; C-: 60%; D: 55%; F: <55%

Notes:

The Instructor reserves the right to seat or move students during the tests.

Students may be asked to show (and leave) their student identification on the desk to take the test. Tests will be graded ONLY upon correct identification of a student.

The Department of Chemistry follows the university policy on academic honesty published in the "Faculty Affairs Handbook" and the "On Campus: The Undergraduate Co-Curricular Affairs Handbook." All tests taken must represent your individual, unaided efforts. To receive or offer information during an examination is cheating. The use of unauthorized supplementary materials during tests is also cheating. A student who cheats on an exam will receive a zero for that exam which cannot be dropped as the lowest grade. Any suspected offenses may also be referred to the Department Chair for appropriate actions.

Suggestions:

Students are strongly encouraged to carefully read and study in depth the topic and available materials before coming to class, and not to wait until the last days to study for tests.

Last day to Withdraw from Class and Receive a "W":

March 29, semester midpoint

The University requires that faculty members must, on a date after the mid-point of the course to be set by the Provost (or his designee):

1. Give a WF to all those students who are on their rolls but no longer taking the class and
2. Report the last day the student attended or turned in an assignment.

Academic Honesty

Students will be expected to maintain the highest standards of academic honesty. With respect to homework assignments, it is expected that no student will turn in work that is not his or her own by copying the work of another student or by using the work or solutions from this course given in previous years. Discussion of

approaches to solving the homework problems after attempting to work the problems independently, however, is permitted and encouraged.

It is expected that during a test or examination, a student will not:

- 1) Accept or use information of any kind from other students.
- 2) Present the work of another student as his or her own.
- 3) Use aids to memory other than those expressly permitted by the examiner.

Following a test or examination, a student will not try to deceive teachers or graders by misrepresenting or altering his or her previous work. In advance of a test or exam, a student will not knowingly obtain access to the exam questions.

Departures from the above standards are contrary to fundamental principles of GSU. Such departures are considered serious offenses for which disciplinary penalties, including suspension and expulsion, can be imposed.

Disability Service:

Students who wish to request accommodation for a disability may do so by registering with the Office of Disability Services. Students may only be accommodated upon issuance by the Office of Disability Services of a signed Accommodation Plan and are responsible for providing a copy of that plan to instructors of all classes in which an accommodation is sought.

V. Final Exam

April 23: Comprehensive Final Exam

Tentative lecture schedule (may be changed as the course progresses)

Week	Date	Chapter	Topic	Lecturer
1	March 5	1-2	Course introduction, Basics	Luo
	March 7	1-2	Methods for measuring ligand binding	Luo
2	12	3	Drug targets	Luo
	14	4	In vitro screen	Luo
3	19		Spring break	
	21		Spring break	
4	26	*	In silico screen	Luo
	28	*	Structure-based drug design	Luo
5	April	2	Hand-on exercise/ Midterm Exam 1	Luo
		4	Disease mechanisms	Luo
6	9	5	Medicinal chemistry	Henry
	11	5	SAR strategy	Luo
7	10	6	in vitro ADME	Luo
	16	6-7	Pharmacokinetics and animal models	Luo
8	18	*	Biologicals/ Midterm Exam 2	Luo
	23		Final exam (time & location to be announced)	

Reference Textbook: Basic Principles of Drug Discovery and Development, 1th edition, by Benjamin Blass.

*: reading materials will be provided.