ILLINOIS
Bioengineering
GRAINGER COLLEGE OF ENGINEERING

BIOE 450: Introduction to Quantitative Pharmacology

Meeting time: Tuesdays and Thursdays, 12:30 – 1:50 PM
Location: 2310 Everitt Laboratory

Credit Hours: 3 (QP1; undergraduate) or 4 (QP2; graduate)
CRN: 79423 (QP1; undergraduate) or 79424 (QP2; graduate)
Semester Offered: Fall

Instructor Information

Name	Professor Andrew M. Smith
Contact Information	smi@illinois.edu
Office Hours	Wednesdays 3:00 – 4:00 PM and by appointment (online or in person)
Office Location	2316 Everitt Laboratory

Course Description

This course introduces interactions between living organisms and substances (drugs) that impact physiology and disease. Concepts will be integrated from equilibrium thermodynamics, kinetics, mass transfer, organic chemistry, biochemistry, and structural biology to understand drug design and function. Students will develop skills in quantitative aspects of medicinal chemistry, pharmacodynamics, and pharmacokinetics through mathematical problem solving and computer simulations. Students will further design and critically assess innovative solutions for current challenges in pharmacology. Materials and content are designed for senior-level undergraduates and graduate students from diverse majors.

Note: This course does not focus on drug discovery, metabolism, or toxicology; students interested in these related concepts should be referred to CHEM 474 and FSHN 480.

Learning Objectives

1. **Apply** terminology from pharmacology and the FDA.
2. **Evaluate and construct** reaction pathway maps and compartment diagrams.
3. **Analyze** drug mechanisms and pathophysiological mechanisms to set up mathematical relationships describing drug equilibrium and transport.
4. **Evaluate** molecular structure to predict oral bioavailability and interface permeability.
5. **Identify** how physicochemical properties of different drug classes dictate function.
6. **Solve** thermodynamics problems to analyze drug pharmacodynamics.
7. **Analyze** biological compartments and interfaces to identify thermodynamic and kinetic parameters related to drug equilibrium and transport.
8. **Solve** pharmacokinetics problems involving multi-compartment models using computer simulations.
9. **Conceptually design** basic technologies to address modern needs in the pharmaceutical industry.
10. **Evaluate** current events and current needs in the pharmaceutical sciences.

Course Format

- Two 80-min classes that mix lecture delivery with interactive problem solving
- Weekly, students are expected to spend 3 hours in class and 6–8 hours outside of class.

Required Prerequisites (equivalence of alternative courses may be allowed with consent of the instructor)

- CS 101 or CS 124
- CHEM 232 or CHEM 236
- MCB 150
- MATH 231

Course Website

Canvas: https://canvas.illinois.edu/courses/62830

Textbook and Reading Materials

No textbooks are required. Some texts will be provided electronically. The following reference texts are recommended for supplementary reading.

- **Drug Delivery – Engineering Principles for Drug Therapy**, Mark Saltzman
  Oxford University Press (2005); ISBN-10: 0195085892; ISBN-13: 978-0195085891
- **An Introduction to Medicinal Chemistry**, Graham Patrick
  Oxford University Press, 5th edition (2013); ISBN-10: 9780199697397; ISBN-13: 978-0199697397
- **Basic Pharmacokinetics and Pharmacodynamics: An Integrated Textbook and Computer Simulations**, Sara Rosebaum
  Wiley, 2nd edition (2016); ISBN-10: 9781119143154; ISBN-13: 978-1119143154

Course Schedule

Wk		Date	Topic (Module #)
1	T	26-Aug	Course overview & pharmacology introduction
	Th	28-Aug	(1) Drug function & classification
2	T	2-Sep	(2) Drug Metrics
	Th	4-Sep	(2) Drug Metrics
3	T	9-Sep	(3) Small drug structure – bond rotation
	Th	11-Sep	(3) Small drug structure – Lipinski's rules problems
4	T	16-Sep	(4) Molecular charge and reaction equilibrium – molecular species fractionation
	Th	18-Sep	(4) Molecular charge and reaction equilibrium – acid/base & charge
5	T	23-Sep	(4) Molecular charge and reaction equilibrium – problem solving
	Th	25-Sep	(5) Multicompartment equilibrium solutions – kidney nephron
6	T	30-Sep	(5) Multicompartment equilibrium solutions – ADME
	Th	2-Oct	(5) Multicompartment equilibrium solutions – volume of distribution
7	T	7-Oct	(5) Multicompartment equilibrium solutions – MATLAB solutions
	Th	9-Oct	(6) Clinical case studies – differential diagnosis
8	T	14-Oct	**EXAM 1**
	Th	16-Oct	(6) Clinical case studies – case 1
9	T	21-Oct	(6) Clinical case studies – case 2
	Th	23-Oct	Projects
10	T	28-Oct	(7) Pharmacokinetics
	Th	30-Oct	Projects
11	T	4-Nov	(7) Pharmacokinetics
	Th	6-Nov	(7) Pharmacokinetics
12	T	11-Nov	(8) Biological compartments & interfaces
	Th	13-Nov	(8) Biological compartments & interfaces
13	T	18-Nov	(9) Small drugs & biologics
	Th	20-Nov	(9) Small drugs & biologics
14	T	25-Nov	No class: Fall Break
	Th	27-Nov	No class: Fall Break
15	T	2-Dec	Projects
	Th	4-Dec	Projects
16	T	9-Dec	**EXAM 2**
	Th	11-Dec	No class: Reading Day

Grading

Homework	30%
Exams (2)	30%
Project*	30%
Attendance & participation**	10%

* Projects: Students will work in teams to analyze new translational concepts in pharmacology culminating in a written document and presentation. Students will also serve as evaluators, assuming roles of representatives from physicians, consumer advocates, industry, FDA, and insurance agencies.

** For graduate students in the QP2 section, an additional assignment will provide 5% of the attendance and participation grade.

Letter Grade Distribution:

≥ 93.00	A
90.00 – 92.99	A–
87.00 – 89.99	B+
83.00 – 86.99	B
80.00 – 82.99	B–
77.00 – 79.99	C+
73.00 – 76.99	C
70.00 – 72.99	C–
67.00 – 69.99	D+
63.00 – 66.99	D
60.00 – 62.99	D–
≤ 59.99	F

Course Policies

Attendance**:** Students are expected to attend every class with the exception of authorized absences or unavoidable emergencies. Roll will be compiled from written attendance logs or Zoom chat comments in the event that a class must meet online.

Course-related communications**:** Course announcements will be sent via Canvas Announcements and Discussions; please check these regularly. For general course questions and information, first consult the syllabus. Use the Canvas Discussion forum for all communications related to class. In case of emergencies, email the instructor at smi@illinois.edu.

Academic Integrity

The university's policy on Academic Integrity can be found in the *Code of Policies and Regulations Applying to All Students* under Article One, Part IV, which can be found at: https://studentcode.illinois.edu/. The following policies support and reinforce that policy.

1. All students are expected to hold the highest standards of scientific and academic conduct. Any form of cheating on graded work in this course is unacceptable and will be dealt with as outlined below in accordance with the *Code of Policies and Regulations Applying to All Students.*
2. It is a requirement that all graded work be entirely your own, and that anything you write using the words of other writers is correctly attributed. Some specific points follow:

   Plagiarism*: On all assignments, exams, and presentations,* all written and verbally communicated content must be your own words, formulated from your understanding of the material, and not copied from any other material. If the work you submit resembles that of another work or that of another student/team (including work from previous offerings of this or other courses), it may be concluded that it was not your original work. Turnitin will be used to determine the degree to which submitted materials resemble previous work. If you use the *ideas and/or opinions* from another author or source, you must provide the citation. That is, using APA format, include a parenthetical reference to the source that provided this information.

Figures, schematics, and graphical content will be used in projects and related materials. These materials may be acquired from the literature or other sources; however, *the source must be cited in all cases*. Describing information (*i.e.*, figure legends) must be paraphrased in your own words.

Direct quotations: Direct quotations should rarely be used in your assignments; they should be used ONLY in the two cases below:

- A definition of a term. In this case, you must put the text in quotes and, using APA format, place a parenthetical reference to the source at the end of the quote.
- A profound statement made by an expert in the field. In this case, you must put the text in quotes and, using APA format, place a parenthetical reference to the source at the end of the quote.

3. Group work will be an important part of this class. On all group assignments and presentations, each group member must contribute demonstrably to the group's effort. Group work cannot be monitored directly, and the appearance of the work is the only means to determine the contribution of each member to the team.

Failure to adhere to these standards may result in a grade of *zero for the entire assignment*, *for all persons involved.*

Illness Policies

All proceedings of this class will follow the recommendations on campus policies provided on the University of Illinois Urbana-Champaign's COVID-19 website. It is strongly recommended that students who feel ill should not come to class.

Emergency response recommendations can be found at the following website: https://police.illinois.edu/em/emergency-response-guide/

Disability Related Accommodations

To obtain disability-related academic adjustments and/or auxiliary aids, students should contact the course instructor and the Disability Resources and Educational Services (DRES) as soon as possible. To contact DRES, you may visit 1207 S. Oak St., Champaign, call 333-4603, e-mail disability@illinois.edu, or go to https://dres.illinois.edu/. If you are concerned that you may have a disability-related condition that is impacting your academic progress, there are academic screening appointments available that can help diagnose a previously undiagnosed disability. You may access these by visiting the DRES website and selecting "Request an Academic Screening" at the bottom of the webpage.

Family Educational Rights and Privacy Act

Any student who has suppressed their directory information under the Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure the protection of the privacy of their attendance in this course. See https://registrar.illinois.edu/academic-records/ferpa/ for more information on FERPA.

Religious Observances

Illinois law requires the University to reasonably accommodate its students' religious beliefs, observances, and practices with regard to admissions, class attendance, and the scheduling of examinations and work requirements. You should examine this syllabus at the beginning of the semester for potential conflicts between course deadlines and any of your religious observances. If a conflict exists, you should notify your instructor of the conflict and follow the procedure at https://odos.illinois.edu/community-of-care/resources/students/religious-observances/ to request appropriate accommodations. This should be completed in the first two weeks of classes.