

Course syllabus for Chemistry 162/262

Drug Design

Class meets: Mon, Wed, Fri 10:00 – 10:50 AM Webb 1100

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Office Hours: Tue and Fri (12:00-1:00 PM) or by appointment
Course website: <http://www.chem.ucsb.edu/~kalju/chem162>

Teaching Assistant: August Estabrook, Chem 1148, x8283 aestabrook@chem.ucsb.edu

Lecture Textbooks:

Required: Richard B. Silverman,
The Organic Chemistry of Drug Design and Drug Action, 2nd edition

The Course:

In Chem 162 students learn principles that govern the process of modern drug discovery and development. Students will follow a path similar to that taken by real-life drug developers by learning important elements of the drug design process in a logical order. Some topics that we focus more extensively are:

- Target validation
- Structure-base drug design
- Enzyme inhibition
- Drug metabolism

Expectations of Students:

- Attendance and taking good lecture notes is expected. Submitting completed assignments in time is required.
- The textbook provides necessary background material. Furthermore, students are expected to read modern drug design-related research literature. Required literature will be available on the course website.
- Honesty and academic integrity must be always preserved. While discussing your ideas with others is encouraged outside the classroom, you must answer the assignment questions individually. No supplemental material should be used during an exam.
- Your grade in the course is based on points you collect from the weekly assignments (10 points each), the mid-term (40 points), the poster presentation (20 points), and the final written research proposal (50 points). Grading will be based on the curve but you have to meet a certain level to get a grade higher than F.
- The course requires that you have a solid understanding of organic chemistry; good background in biochemistry and physical chemistry will be very helpful.

Study tips:

- Read the relevant textbook material and required reading **before** the class meets. I like to interact with students during our meetings and you enjoy the lectures more if you can think along.
- Review (or rewrite) your class notes the same day and supplement them with material from the textbook and other resources (optional reading, Internet). Ask for help if something remains unclear.
- This course is not about memorization of names, reactions, or facts. It is about understanding the process, its principles and methods. You should demonstrate good understanding of the material in when answering assignment questions and the midterm problems. Your creativity and originality are highly important for getting a high score in the final written proposal.

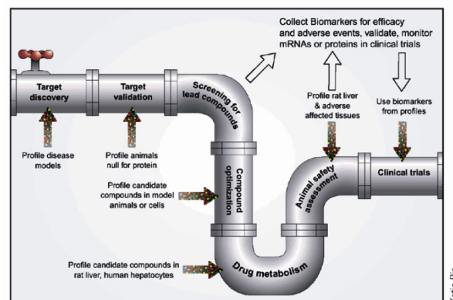
Good luck! — Kalju

Chem162/262**Schedule for the Spring 2004**

March 29 th	M	Overview of the course. History of drug design	
March 31 st	W	Current trends and future of drug design. Diseases	
April 2 nd	F	Target validation.	
April 5 th	M	Biomolecular interactions. Receptors and enzymes.	
April 7 th	W	Lead discovery and modification. Pharmacophores	First assignment due
April 9 th	F	Pharmacokinetics (ADME)	
April 12 th	M	Enzyme mechanisms	
April 14 th	W	Enzyme kinetics and inhibition	Second assignment due
April 16 th	F	Enzyme inhibition. Reversible inhibitors, TSA	
April 19 th	M	Enzyme inhibition. Irreversible inhibitors. Mechanism-based inactivators	
April 21 st	W	Drug-receptor interactions. Pharmacodynamics.	Third assignment due
April 23 rd	F	Structure based drug design: Overview	
April 26 th	M	Structure-based drug design: Theoretical foundations	
April 28 th	W	Structure-based drug design: Docking, FEP	Fourth assignment due
April 30 th	F	Structure-based drug design: Virtual screening	
May 3 rd	M	Medicinal and Combinatorial Chemistry	
May 5 th	W	Mid-Term Examination (45 minutes)	
May 7 th	F	QSAR: Theoretical foundations, applications	Fifth assignment due
May 10 th	M	Drug metabolism and toxicity	
May 12 th	W	Drug metabolism: Pathways for deactivation	Sixth assignment due
May 14 th	F	Prodrugs. Drug delivery systems	
May 17 th	M	Pharmacogenomics	
May 19 th	W	Pharmacogenomics	Seventh assignment due
May 21 st	F	Nucleic acids as therapeutics	
May 24 th	M	Proteins as therapeutics	
May 26 th	W	Animal studies and clinical trials	Eight assignment due
May 28 th	F	Intellectual property. Drug approval	
May 31 st	M	Memorial Day:	
June 2 nd	W	Pharmaceutical industry: Strategic management	Ninth assignment due
June 4 th	F	Posters. Noon–2:00 PM, Chemistry breezeway	
June 7 th	M	Written proposals due	

Assignments (will be posted on Wednesday week before the due date)

1. Target validation
2. Biomolecular interactions. Pharmacokinetics
3. Enzyme mechanisms and kinetics
4. Enzyme inhibition and inactivation
4. Structure-based drug design
5. Medicinal and combinatorial chemistry, screening
6. QSAR
7. Drug metabolism, prodrugs, drug delivery
8. Pharmacogenomics
9. Nucleic acids and proteins as therapeutics



It is not necessary to know all the material in the textbook for this course. The following pages are most relevant for each topic that we discuss. However, interested students are encouraged to read more. N/A means that the textbook does not offer adequate coverage; students should use posted research literature as a source of additional information.

History of drug design	1-11
Current trends and future of drug design. Diseases	N/A
Target validation	N/A
Biomolecular interactions. Receptors and enzymes.	122-137
Lead discovery and modification. Pharmacophores	11-34;
Pharmacokinetics (ADME)	51-66
Enzyme mechanisms	174-190
Enzyme kinetics and inhibition	227-240
Enzyme inhibition. Reversible inhibitors, TSA	241-264
Enzyme inhibition. Irreversible inhibitors. Mechanism-based inactivators	274-302
Drug-receptor interactions. Pharmacodynamics	137-159, suggested: 159-165
Structure based drug design: Overview	78-87; 268-272
Structure-based drug design: Theoretical foundations	N/A
Structure-based drug design: Docking, FEP	82-83
Structure-based drug design: Virtual screening	N/A
Medicinal and Combinatorial Chemistry	34-50
QSAR: Theoretical foundations, applications	66-78
Drug metabolism and toxicity	406-414
Drug metabolism: Pathways for deactivation	415-448
Prodrugs. Drug delivery systems	498-528
Pharmacogenomics	N/A
Pharmacogenomics	N/A
Nucleic acids as therapeutics	324-328, 342-359
Proteins as therapeutics	N/A
Animal studies and clinical trials	N/A
Intellectual property. Drug approval	N/A
Pharmaceutical industry: Strategic management	N/A