Course syllabus for Chemistry 162A / 262A

Drug Design (Winter 2009)

Class meets: Mon, Wed, Fri **12:00 – 12:50** AM **Phelps 1444**

Instructor: Professor *Kalju Kahn*, Office: PSB-N 2623
E-mail: kalju@chem.ucsb.edu Phone: (805) 893-6157
Office Hours: Tue 12:30-1:30 and Thu 12:30-1:30 or by appointment
Course website: http://www.chem.ucsb.edu/~kalju/chem162

Teaching Assistant: *Robert Levenson*, Office Chem 1317

Lecture Textbook: 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 in 162A are:

- Target identification and validation
- Chemical libraries and screening
- Receptor mechanisms and receptor targeting
- Ligand-based drug design

Expectations of Students:

- Attendance and taking good lecture notes is expected. Submitting completed assignments in time is required.
- The textbook provides some 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 final exam (50 points), and the 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 basic biology and organic chemistry; good background in biochemistry and physical chemistry will be very helpful.
- No student shall give, sell, or otherwise distribute to others or publish any electronically available course materials or recordings made during any course presentation without the written consent of the instructor.

Study tips:

- I am posting lecture note slides on-line before the class meets so that you can focus on following my talk. The slides are mainly illustrative and you need to follow the lecture in order to fully understand the topics I cover.
- Come in class prepared. 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 when answering assignment questions and the exam 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 Winter 2009**

Jan 5th	M	Overview and history of drug design	
Jan 7th	W	Rational drug design: overview of approaches	
Jan 9th	F	Current trends and future of drug design. Diseases.	
Jan 12th	M	Target Identification and Validation: Principles	
Jan 14th	W	Target Validation: Pre-genomic methods	
Jan 16th	F	Target Validation: Post-genomic methods	
Jan 19th	M	Martin Luther King, Jr.'s Birthday	
Jan 20th	M	Target Validation: Bioinformatics	**First assignment due**
Jan 21st	W	Tutorial in SGI lab (Chem 1153): Target identification from microarray data	
Jan 26th	M	Enzymes as drug targets	
Jan 28th	W	Receptors as drug targets: Overview of biosignaling	**Second assignment due**
Jan 30th	F	Receptors as drug targets: Ion channels	
Feb 2nd	M	Receptors as drug targets: G-protein coupled receptors	
Feb 4th	W	Experimental characterization of membrane-bound receptors	**Third assignment due**
Feb 6th	F	Nuclear hormone receptors	
Feb 9th	M	Midterm Exam	
Feb 11th	W	Chemical libraries and combinatorial chemistry	
Feb 13th	F	Principles of assay development	
Feb 16th	M	Presidents' day	
Feb 18th	W	High-throughput screening for lead identification	**Fourth assignment due**
Feb 20th	F	General strategies for lead optimization	
Feb 23rd	M	Ligand-based drug design and optimization	
Feb 25th	W	Ligand-based drug design and optimization	**Fifth assignment due**
Feb 27th	F	Tutorial in SGI lab (Chem 1153): Ligand building and modeling	
Mar 2nd	M	Fragment-based drug design and optimization	
Mar 4th	W	QSAR: Overview	**Sixth assignment due**
Mar 6th	F	Tutorial: Practical QSAR: tutorial in the SGI lab (Chem 1153)	
Mar 9th	M	QSAR: Technical Details	
Mar 11th	W	Comparative Molecular Field Analysis	
Mar 13th	F	Open	**Written draft proposals due**

Assignments
(will be posted on Wednesday one week before the due date)
1. Diseases and targets
2. Target validation
3. Receptors: general features
4. Assay development and library design
5. Pharmacophores and molecular similarity
6. Molecular properties, ligand-based optimization