

# Course syllabus for Chemistry 162A / 262A

## Drug Design (Fall 2009)

Class meets: Mon, Wed, Fri                      11:00 – 11:50 AM                      Phelps 3505

**Instructor:** Professor *Kalju Kahn*, Office: PSB-N 2623  
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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*, 2<sup>nd</sup> 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
- Receptor mechanisms and receptor targeting
- Chemical libraries and screening
- 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**

|                      |   |   |                              |
|----------------------|---|---|------------------------------|
| Sep 25 <sup>th</sup> | F | Overview and history of drug design   |                              |
| Sep 27 <sup>th</sup> | M | Rational drug design: overview of approaches                                |                              |
| Sep 30 <sup>th</sup> | W | Current trends and future of drug design. Diseases.                         |                              |
| Oct 2 <sup>nd</sup>  | F | Target Identification and Validation: Principles                            |                              |
| Oct 5 <sup>th</sup>  | M | Target Validation: Pre-genomic methods                                      |                              |
| Oct 7 <sup>th</sup>  | W | Target Validation: Post-genomic methods                                     | <b>First assignment due</b>  |
| Oct 9 <sup>th</sup>  | F | Tutorial in SGI lab (Chem 1153): Target identification from microarray data |                              |
| Oct 12 <sup>th</sup> | M | Enzymes as drug targets   |                              |
| Oct 14 <sup>th</sup> | W | Receptors as drug targets: Overview of biosignaling                         | <b>Second assignment due</b> |
| Oct 16 <sup>th</sup> | F | Receptors as drug targets: Ion channels                                     |                              |
| Oct 19 <sup>th</sup> | M | Receptors as drug targets: G-protein coupled receptors                      |                              |
| Oct 21 <sup>st</sup> | W | Experimental characterization of membrane-bound receptors                   | <b>Third assignment due</b>  |
| Oct 23 <sup>rd</sup> | F | Nuclear hormone receptors   |                              |
| Oct 26 <sup>th</sup> | M | <b>Midterm Exam</b>   |                              |
| Oct 28 <sup>th</sup> | W | Combinatorial chemistry   |                              |
| Oct 30 <sup>th</sup> | F | Chemical libraries  |                              |
| Nov 2 <sup>nd</sup>  | M | Principles of assay development   | <b>Fourth assignment due</b> |
| Nov 4 <sup>th</sup>  | W | High-throughput screening for lead identification                           |                              |
| Nov 6 <sup>th</sup>  | M | General strategies for lead optimization                                    |                              |
| Nov 9 <sup>th</sup>  | M | Ligand-based drug design and optimization                                   | <b>Fifth assignment due</b>  |
| Nov 11 <sup>th</sup> | W | <b>Veteran's day</b>  |                              |
| Nov 13 <sup>th</sup> | F | Tutorial in SGI lab (Chem 1153): Ligand building and modeling               |                              |
| Nov 16 <sup>th</sup> | M | Ligand-based drug design and optimization                                   |                              |
| Nov 18 <sup>th</sup> | W | Fragment-based drug design and optimization                                 | <b>Sixth assignment due</b>  |
| Nov 20 <sup>th</sup> | F | QSAR: Overview  |                              |
| Nov 23 <sup>th</sup> | M | QSAR: Technical Details   |                              |
| Nov 25 <sup>th</sup> | W | Tutorial: Practical QSAR: tutorial in the SGI lab (Chem 1153) Analysis      |                              |
| Nov 27 <sup>th</sup> | F | <b>Thanksgiving Holiday</b>   |                              |
| Nov 30 <sup>th</sup> | M | Comparative Molecular Field Analysis  |                              |
| Dec 2 <sup>nd</sup>  | W | Nucleic Acid Drugs  |                              |
| Dec 4 <sup>th</sup>  | F | Course Review and Evaluation  |                              |

**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

