Course syllabus for Chemistry 162/262

Drug Design

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

Instructor: Professor Kalju Kahn, Office: PSB-N 1511,
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Phone: (805) 893-6157
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 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
- Enzyme inhibition
- Structure-base drug design
- 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 29th M  Overview of the course. History of drug design
March 31st W  Current trends and future of drug design. Diseases
April 2nd F  Target validation.
April 5th M  Biomolecular interactions. Receptors and enzymes.
April 7th W  Lead discovery and modification. Pharmacophores
April 9th F  Pharmacokinetics (ADME)
April 12th M  Enzyme mechanisms
April 14th W  Enzyme kinetics and inhibition
April 16th F  Enzyme inhibition. Reversible inhibitors, TSA
April 19th M  Enzyme inhibition. Irreversible inhibitors. Mechanism-based inactivators
April 21st W  Drug–receptor interactions. Pharmacodynamics.
April 23rd F  Structure based drug design: Overview
April 26th M  Structure-based drug design: Theoretical foundations
April 28th W  Structure-based drug design: Docking, FEP
April 30th F  Structure-based drug design: Virtual screening

May 3rd M  Medicinal and Combinatorial Chemistry
May 5th W  Mid-Term Examination (45 minutes)
May 7th F  QSAR: Theoretical foundations, applications

May 10th M  Drug metabolism and toxicity
May 12th W  Drug metabolism: Pathways for deactivation
May 14th F  Prodrugs. Drug delivery systems
May 17th M  Pharmacogenomics
May 19th W  Pharmacogenomics
May 21st F  Nucleic acids as therapeutics
May 24th M  Proteins as therapeutics
May 26th W  Animal studies and clinical trials
May 28th F  Intellectual property. Drug approval

May 31st M  Memorial Day:
June 2nd W  Pharmaceutical industry: Strategic management
June 4th F  Posters. Noon–2:00 PM, Chemistry breezeway

June 7th 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.

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<tr>
<td>History of drug design</td>
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<tr>
<td>Current trends and future of drug design. Diseases</td>
<td>N/A</td>
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<td>Target validation</td>
<td>N/A</td>
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<td>Biomolecular interactions. Receptors and enzymes.</td>
<td>122-137</td>
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<td>Enzyme mechanisms</td>
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<td>Enzyme kinetics and inhibition</td>
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<td>Enzyme inhibition. Irreversible inhibitors. Mechanism-based inactivators</td>
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<tr>
<td>Drug–receptor interactions. Pharmacodynamics</td>
<td>137-159, suggested: 159-165</td>
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<tr>
<td>Structure based drug design: Overview</td>
<td>78-87; 268-272</td>
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<td>Structure-based drug design: Theoretical foundations</td>
<td>N/A</td>
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<td>Structure-based drug design: Docking, FEP</td>
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<td>Structure-based drug design: Virtual screening</td>
<td>N/A</td>
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<td>Medicinal and Combinatorial Chemistry</td>
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<td>QSAR: Theoretical foundations, applications</td>
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<td>Prodrugs. Drug delivery systems</td>
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<td>Pharmacogenomics</td>
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<td>Nucleic acids as therapeutics</td>
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