CH4800/6490 – Part 1
Spring Semester 2005

Instructor: Dr. Dallas K. Bates
e-mail: dbates@mtu.edu

Class time and place: Class meets TR 3-4:40 in ChemSci 404.

Office Hours: 10:00-10:30 am MWF and by arrangement

Office: 19-708A


Useful REFERENCE texts:
The Merck Index;
D. Lednicer, The Organic Chemistry of Drug Synthesis (5 - volume set);
M.E. Wolff, Burger’s Medicinal Chemistry and Drug Discovery (6 – volumes)

Software: HyperChem v6.x, ChemDraw

Grading:

This year Pharm. Chem. 1 and 2 are being offered for the first time and in an abbreviated, combined form this semester. Next year each will be a one semester stand-alone course. I will be teaching the first part of the course (Pharm. Chem. 2, actually) and Professor Murthy will teach the second portion. You will be assigned a grade for each component separately and Professor Murthy and I will meet at the end of the semester to combine our grades to determine your final course grade.

At the end of the course, each member of the class will prepare and present a poster related to topics covered during both course parts. Details will be provided later. This poster will be only a small contribution to your final grade and will be used mainly to determine whether borderline grades should be bumped to the next level.

For Part 1, graded material will consist of

Homework 25 %
Quizzes 50 %
Final (during 7th week) 25 %

If you must miss a class, email me prior to class indicating the reason for your absence. Quizzes missed due to an unexcused absence are graded as 0.
TOPICS

Lecture material, homework problems and in-class group problem assignments will cover the following topics: *(This is a work in progress!)*

- Medicinal Chemistry – Historical Context
  - Lead compounds and their sources
- Introduction to molecular modeling
  - Conformations of molecules
  - Torsion angles
  - Molecular energies
  - 1- and 2-dimentional potential energy surfaces
- Thermodynamics: conformer populations
- Kinetics: molecular rotations and other assorted molecular gyrations
- Bio-active conformations
- Molecular mechanics
- Pharmacophore-based drug design
  - The pharmacophore
  - Functional group modification
  - Molecular mimicry
  - SAR
  - Structure modification
- Receptor- based drug design
  - Receptors (Chapter 2)
  - Docking

The *Blue Book of Useful Med. Chem. Information*

A hand-written (no exceptions) “Blue Book of Useful Med. Chem. Information” may be used on quizzes and the final exam. You may include any information in the blue book. The ONLY source that may be used on tests and quizzes is your blue book and all information in the blue book must be hand-written by the individual using it. You can add new material to your bluebook at anytime- plan ahead for expansion of various sections during the semester.

CH4800/6490 information will be posted on the CH4800 course web page (go to the MTU Chemistry homepage, click on “course” in the menu on the left side of the page, then click on CH4800).

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