CH4120
Fall Semester 2005

Instructor:            Dr. Dallas K. Bates
demail:               dbates@mtu.edu

Class time and place: To be determined
(email me your current/class work schedule)

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

Office:               19-708A

Text:                The Organic Chemistry of Drug Design and Drug Action,  
                     2004. ISBN: 0-12-643732-7

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, Molecular Conceptor 2

Class Format

This year Pharm. Chem. 2 is being offered for the first time in a semester format. This course is a cornerstone course in the Pharmaceutical Chemistry degree program approved last year. However, enrollment is expected to be small for the next two offerings until majors reach the 3rd year in the program. Consequently, the format for these initial offerings will be somewhat different than the typical lecture format. We will meet for lecture periodically, but you will also utilize the self-paced software package Molecular Conceptor for the first portion of the course. This software is located on PC05 in the Chemistry Computer Lab.

We will meet once weekly (after the first week) to discuss material covered in the software. These classes are intended to provide a forum to discuss your questions, work on problems utilizing material covered in the software, and for me to ask you questions to gauge your understanding of the material covered. A series of questions for several chapters of Molecular Conceptor are provided on the CH4120 web page; use these as a guide to covering and reviewing material in the software.
When we have completed Molecular Conceptor and Hyperchem problem sets, the class will turn to case studies in drug design using recent articles from the Journal of Medicinal Chemistry. There will also be an organic synthesis component this part of the course.

Grading:

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.

Graded material will consist of

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<td>Homework</td>
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<td>Quizzes</td>
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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

Some of the topics we will discuss include:  
(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-dimesntional 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.

NOTE:

Periodically, information about CH4120 will be posted on the CH4120 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 CH4120. Check it once in a while for new material. I will email you if I post dated, graded material to the page.

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*MTU complies with all federal and state laws and regulations regarding discrimination, including the Americans with Disabilities Act. If you have a disability and need a reasonable accommodation for equal access to education or services at MTU, please call Gloria Melton at 72212. For other concerns you may contact your academic advisor, department chair, or the Affirmative Action Office.*