

# Principles of Medicinal Chemistry II (MCH 402/502)

**Lecture Schedule:** Tuesdays and Thursdays, 9:30 - 10:50 AM, Room 114 Hochstetter, North Campus

**Instructor:** Prof. Thomas Kalman, Ph.D., [tkalman@buffalo.edu](mailto:tkalman@buffalo.edu)

**Office hours:** Wednesdays 9:30 AM – 11:30 AM in 455 Cooke

**Guest Lecturer:** Dr. Wojciech Krzyzanski, [wk@buffalo.edu](mailto:wk@buffalo.edu)

**Teching Assistant:** Harsh Jain, [hvjain@buffalo.edu](mailto:hvjain@buffalo.edu)

**Computer Programs Available:** Wednesdays 5:30 PM – 7:00 PM in 139 Hochstetter with supervision;  
without supervision: 24/7 if the room is not occupied by another class.

**Text:** **The Organic Chemistry of Drug Design and Action, Silverman, R.B. 2nd Ed., 2004, Chapters 7 & 8.**  
Additional materials are made available on **UBlearns** and discussed in class (see also **Library Reserve** below).

**Softwares:** 3D-structures of selected drugs and drug-target complexes will be visualized using **RasTop 2.1**; students should download the "standard package" from: <http://www.geneinfinity.org/rastop/>. Some animations will use **Protein Explorer 2.45beta** (<http://molvis.sdsc.edu/protexpl/frntdoor.htm>), requiring **MDL Chime 2.6 SP6** (<http://www.mdlchime.com/>) and **Netscape 7.2 (or 7.1)**. These should be installed on laptops/notebooks/PCs. Selected materials from the **Molecular Conceptor Courseware** will be used to enhance the learning experience.

**Examination Policy:** Students must take examinations when scheduled, except when excused for acceptable cause, such as a documented illness (doctor's certificate needed). A student must notify the instructor ***by e-mail before*** an examination, if (s)he is unable to take a scheduled examination, ***and obtain approval*** from the instructor. Any student who is not excused from a scheduled examination will receive a zero for the missed examination. No make-up exams are given, except for those officially excused prior to the exam.

**Grading Policy for MCH403:** The final grade is based on two 90-min examinations (30% each), and a 3-hr final exam (40%) on the new material not covered by a previous exam (***not*** cumulative). In addition, take-home exercises on 3D-structures of drug-target complexes can earn extra bonus points to be added to the exam results. Plus/minus grades are given, approximating the following ranges for scores of a possible 100 points total:

**85-100: A- to A    71-84: B- to B+    61-70: C- to C+    51-60: D to D+    =<50: F**

**Grading Policy for MCH502:** In addition the three examinations discussed above, constituting 90% of the total grade, graduate students are required to write term paper on topics selected from a list after the 1st exam. It is due on 4/22 Tuesday, 9:30 AM, graded on a scale of 1 – 10, accounting for 10% of the final grade.

**Student's Responsibilities:** Learning is the student's responsibility. ***Attendance is required!*** The examination questions are based on ***all the material discussed in class, the materials posted on UBlearns, and any additional reading material.***

**Course Content and Goals:** "Drug Metabolism" and "Prodrugs" (Silverman's Chapters 7 & 8) are covered as a continuation of **MCH 401/501**. In addition, fundamentals of drug action, including drug disposition (ADME), principles of pharmacokinetics, membrane structure and function, will be reviewed, and selected drug classes are discussed with a focus on the molecular mechanisms of action of representative drugs. Emphasis is placed on drug-target interactions at the molecular level examined using 3D-visualization techniques, which the students will learn to use. In this course, the medicinal chemistry topics are integrated with relevant topics in biochemistry, physiology, pharmacology and structural biology. There will be an extensive use of internet sources of information.

**Library Reserve (Reference Textbooks and Resources):**

The Organic Chemistry of Drug Design and Action, Silverman, R.B. 2nd Ed., 2004.

Wilson and Giswold's Textbook of Organic Medicinal & Pharmaceutical Chemistry, Block & Beale, 11th Ed. 2004.

Foye's Principles of Medicinal Chemistry, Williams, D.A. & Lemke, T.L., Eds. 5th Ed., 2002.

Burger's Medicinal Chemistry and Drug Discovery, Abraham, D.J., Ed. 6th Ed., 2003. Available online for UB students and faculty: <http://www.mrw.interscience.wiley.com/bmcdd/>