

# Essentials of Medicinal Chemistry

CHM 310

Fall Term 2015 (2nd 7 weeks)

MWF 11:30 am – 12:20 am

Dow L2

Dr. Jeff Turk

KSC 246

Office Hours: MWF 8:30 am – 9:30 am; TTh 10:30 am – 11:30 am, or by appointment

phone: (989) 463-7362

[turk@alma.edu](mailto:turk@alma.edu)

## Supplies (required)

Textbooks:

An Introduction to Medicinal Chemistry, 5th Edition

Graham L. Patrick (Oxford Press 2015)

Textbook Companion Website: <http://global.oup.com/uk/orc/chemistry/patrick5e/>

## Optional Supplies

Molecular model set

Course Website: <http://DrTChemistry.com>

Office Hours: The office hours above are times during each week that I make myself available for you. If the times listed do not coincide with your availability, please let me know in class or contact me via email so we can arrange an appropriate meeting time. Among other things, please use these if you are having difficulties answering the problems at the end of each chapter or with any other course content.

I have 7 weeks to teach medicinal chemistry - an advanced topic. So what information do I cover? The “Essentials...” That’s my task during this 7 week course; to give you the “cream off the top of the cappuccino...”, as a colleague of mine once spoke. Medicinal Chemistry is a broad discipline that combines organic chemistry, biochemistry, physiology, microbiology, cell biology and pharmacology. In a nut-shell, it is the study of drug design and the molecular mechanisms by which drugs interact with the body. It may seem like a BIG cup of cappuccino, but most or all of you will find that the courses you’ve taken so far will have been excellent preparation for this one.

We will be moving through the book at a pretty good clip, so make sure you keep up! Although we’ll be using the textbook as our primary guide, there are some topics I will stress more than

others and some I will skip entirely - so make sure you are paying attention in class. There are LOTS of drug names and scientific/medical terminology that we will not discuss - don't get bogged down by these when you are reading. Remember - if I don't talk about it in class, you won't need the information for an exam or quiz.

The use of computers to aid in drug design is a growing trend, and for some therapeutic applications it is the primary means of design. As such, there are three class periods where we will be using laptop computers to help us build/download and analyze molecules and to calculate/predict their drug-like properties. The first in class session will comprise mostly of training and introductory exercises. If you are unable to complete the assignments in class, the computers will be available two afternoons that week. The last two days of class will comprise the remaining computer exercises; all exercises/assignments will be completed in class.

There are problems at the end of each chapter that are great practice, and for even more practice, the companion website for the textbook has LOTS of multiple choice questions and answers. However keep in mind that only those problems that parallel to what we cover in class are relevant.

Examinations and Grading: Exam content will come from material covered during our class meetings, assignments and handouts, which for many chapters will not represent all the content introduced in the textbook. There will one mid-term and one comprehensive final exam. There will also be four quizzes that will account for approximately 10% of your grade - these will be taken directly from the online multiple-choice questions. Your course grade will be determined by the total points acquired during the term and may be curved to reflect your standing in the class. This syllabus is tentative and lecture topics may change, however exam days/times will not. Re-grading requests must be made within 48 hours of receipt of the exam. Academic dishonesty will be dealt with vigorously and will result in a zero for the exam/assignment.

Midterm Exam:	100 pts. (30%)
Comprehensive Final Exam:	150 pts. (45%)
Computer Assignments	40 pts. (12%)
Quizzes:	40 pts. (12%)
Total =	330 pts.

## Tentative Lecture Schedule

Asterisks\* indicate laptop computers will be made available in KSC 261 from 1 PM to 4 PM.

<u>Date</u>	<u>Itinerary (Chapter)</u>	<u>Recommended Textbook Problems</u>
Oct 26, 28	Drugs and Drug Targets: An Overview (1.1 – 1.3.6)	1 - 7, 9
	Proteins: Structure and Function (2.1 - 2.4, 2.7 - 2.7.3)	1 - 6
	Enzymes: Structure and Function (3.1 - 3.5.4)	2 - 4
30	Enzymes as Drug Targets (7.1 - 7.5)	1 - 5 (for 2, see p. 600)
Nov 2	Receptors: Structure and Function (4 - 4.7.2)	1 - 4
4	Receptors as Drug Targets (8.1 - 8.3.2)	1 - 4, 6, 7
6	Nucleic Acids: Structure and Function (6.1 - 6.1.3, 6.2.1)	1
9	Nucleic Acids as Drug Targets (9.1, 9.3 - 9.3.6)	2
11	Pharmacokinetics (11.1 - 11.3.6, 11.4 - 11.5, 11.7.4)	1 - 8
13	Pharmacokinetics, continued	
16*	Molecular Visualization, Part A	
18*	Exam 1	
20	Drug Discovery: Finding a Lead (12.1 - 12.3.5, 12.4 - 12.7)	1, 2, 4, 5
23	Drug Design: Structure Activity Relationships (13.1 - 13.1.16)	1 - 10
25	Drug Design: Pharmacophores (13.2)	
	Drug Design: Optimizing Target Interactions (13.3 - 13.3.11)	
27	Thanksgiving Recess	
30	Drug Design: Optimizing Access to the Target (14.1 - 14.6.8)	2 - 7, 9, 11
Dec 2	Drug Design: Peptidomimetics (14.9 - 14.9.2)	
4	Getting the Drug to the Market (15.1 - 15.1.4.4)	
	Quantitative Structure-Activity Relationships (18.1 - 18.4)	1, 2, 4 - 6
7	QSAR, continued	
9	Molecular Visualization, Part B	
11	Molecular Visualization, Part C	
15	Final Exam, 9 - 11 a.m.	