

**Drug Design I - PHA 6447**

Fall 2021

**Course Coordinator:**

Guangrong Zheng, Ph.D.  
Associate Professor

**Phone:** 294-8953

**Room:** BG-022C

**Email:** zhengg@cop.ufl.edu

**Class Time:** MWF 3:00-5:00 pm. Most of the lectures will be 1-hour in length and start at 3 pm. Any changes to class times and dates will be communicated in advance.

**Classroom:** Lectures and exams will be held in Communicore Rooms. Please pay close attention to assigned classroom locations listed on the schedule (next page).

**Canvas Website:** Course materials, including pre-reading materials/handouts, and announcements can be found on the Canvas Website that is associated with this course.

**Description:** Outline of how relevant disciplines impact on the development of a new drug product from the discovery of a new active lead compound to its final refinement as a commercial product. Contributions of Organic Chemistry, Biochemistry, Metabolic Chemistry, Physical Chemistry, Analytical Chemistry, and Pharmacological Chemistry are discussed. Students will gain a general understanding of the drug design process.

**Reference Text:**

- 1) R. B. Silverman, *The Organic Chemistry of Drug Design and Drug Action*, 3<sup>rd</sup> Edition.
- 2) V. F. Roche, S. W. Zito, T. L. Lemke, and D. A. Williams, *Foye's Principles of Medicinal Chemistry*, 8<sup>th</sup> Edition.
- 3) L. L. Brunton, R. Hilal-Dandan, and B. C. Knollmann, *Goodman & Gilman's: The Pharmacological Basis of Therapeutics*, 13<sup>th</sup> Edition. Ebook link: <https://accesspharmacy.mhmedical.com/book.aspx?bookid=2189>

**Pre-requisites:** Advanced Undergraduate Organic Chemistry; Undergraduate Biochemistry.

**Learning Objectives:**

1. Students should acquire knowledge of organic chemistry, organic/bioorganic reaction mechanisms, prodrugs and some chemical synthesis related to drug molecules.
2. Students should gain a fundamental understanding of the chemical and physiochemical properties of therapeutic agents.
3. Students should learn the fundamentals of drug targets/receptors, pharmacology, pharmacophores, ADME principles, drug metabolism and toxicology.
4. Students should attain specific medicinal chemistry competencies that are required for critical thinking and problem solving skills in the acquisition of this knowledge base.
5. These medicinal chemistry competencies will establish the foundation for your continuing professional education and development.

## COURSE CALENDAR

<u>Date</u>	<u>Subject</u>	<u>Lecturer</u>
Aug. 25	Overview of Med. Chem. / Basic & Organic Chemistry	Huigens (C1-17)
27	Basic & Intermediate Organic Chemistry	Huigens (C1-07)
30	Basic & Intermediate Organic Chemistry	Huigens (C1-03)
Sep. 1	Basic & Intermediate Organic Chemistry	Huigens (C1-03)
3	Med. Chem. Literature Search	Mottinelli (C1-07)
<b>6</b>	<b>Labor Day – NO CLASS</b>	--
8	Miscellaneous Subjects	Mottinelli (C1-03)
10	Basic & Intermediate Organic Chemistry	Huigens (C1-07)
13	Basic & Intermediate Organic Chemistry	Huigens (C1-03)
15	Basic & Intermediate Organic Chemistry	Huigens (C1-03)
17	Introduction to Drug Absorption, Distribution & Elimination	James (C1-07)
20	Introduction to Pathways of Drug Metabolism	James (C1-03)
<b>22</b>	<b>Exam I</b>	<b>Huigens Admin.</b> (C1-03)
24	Predicting Water Solubility	McCurdy (C1-07)
27	Ionization of Drugs (Acid/Base)	McCurdy (C1-03)
29	Ionization of Drugs (Acid/Base)	McCurdy (C1-17)
Oct 1	Drug/Chemical Stability	McCurdy (C1-07)
4	Quantitative Aspects of Drug Action	Aldrich (C1-03)
6	Introduction to Pharmacology	Aldrich (C1-03)
<b>8</b>	<b>Homecoming – NO CLASS</b>	--
11	Introduction to Pharmacology	Aldrich (C1-03)
13	Drug-Receptor Interactions (Forces)	Aldrich (C1-03)
15	Amino Acids and Peptides	Aldrich (C1-07)
18	Drug Targets	Aldrich (C1-03) (be tested in Exam III)
<b>20</b>	<b>Exam II</b>	<b>McCurdy Admin.</b> (C1-03)
22	Receptor Pharmacology	Aldrich (C1-07)
25	Enzyme Mechanisms	Aldrich (C1-03)
27	Mechanisms of Inhibition	Aldrich (C1-17)
29	Hit-to-Lead / SAR	Zheng (C1-07)
Nov. 1	Hit-to-Lead / SAR	Zheng (C1-03)
3	Hit-to-Lead / SAR	Zheng (C1-03)
5	Hit-to-Lead / SAR	Zheng (C1-07)
<b>8</b>	<b>Exam III</b>	<b>Zheng Admin.</b> (C1-03)
10	Cytochrome P450 Enzymology & Drugs that Target P450 I	James (C1-03)
12	Cytochrome P450 Enzymology & Drugs that target P450 II	James (C1-07)
15	Drugs that target P450	James (C1-03)
17	Importance of Stereochemistry	James (C1-03)
19	“Phase II” Pathways of Drug Metabolism	James (C1-07)
22	Reactive/Toxic Metabolites of Drugs I	James (C1-17)
<b>24-26</b>	<b>Thanksgiving Break – NO CLASS</b>	--
29	Reactive/Toxic Metabolites of Drugs II	James (C1-03)
Dec. 1	Carcinogen Bioactivation I	Xing (C1-03)
3	Carcinogen Bioactivation II	Xing (C1-07)
6	Drug–Drug Interactions	Xing (C1-03)
8	Drug–Herb Interactions	Xing (C1-03)
<b>10</b>	<b>Exam IV</b>	<b>Xing Admin.</b> (C1-07)

## **EXAMS AND GRADING:**

### **Format:**

The format of the course will involve lectures using combinations of Power Point presentations, chalk-board presentations, overhead projection and handouts to deliver the materials.

### **Evaluation:**

The students will be evaluated in FOUR exams each worth 25% of the final points for the course. They will involve structure, short or numerical answers. Exams will be returned to students but copies of the exams will be kept by the faculty for three years. Students will be allowed to review their exams to verify their scores with the faculty.

Grading will be on a point basis with >90 (A), >87 (A-), >83 (B+), >80 (B), >77 (B-), >73 (C+), >70 (C), >67 (C-), >63 (D+), >60 (D), >57 (D-), >53 (E). *There will be no make-up exams.*

### **Miscellaneous:**

Class attendance is not mandatory. However, the student will be tested on the lecture material and in-class handouts, which, for the most part, are not covered in precisely the same way in any available textbook.

Students requesting classroom accommodation must first register with the Dean of Students Office. The Dean of Students Office will provide documentation to the student who must then provide this documentation to the Instructor when requesting accommodation.

Students are expected to complete assignments and take exams with integrity. Academic dishonesty will not be tolerated. If a student commits academic dishonesty, the academic penalty will be a failing grade in the course. The UF policies and procedures on academic dishonesty will be followed.