

**Drug Design I - PHA 6447**

Fall 2022

**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 Building C1-007**.

**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 (Absorption, Distribution, Metabolism, and Excretion) 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. 24	Overview of Med. Chem. / Basic & Organic Chemistry	Huigens
26	Basic & Intermediate Organic Chemistry	Huigens
29	Basic & Intermediate Organic Chemistry	Huigens
31	Basic & Intermediate Organic Chemistry	Huigens
Sep. 2	Med. Chem. Literature Search & Miscellaneous Subjects	Wu
<b>5</b>	<b>Labor Day – NO CLASS</b>	--
7	Basic & Intermediate Organic Chemistry	Huigens
9	Basic & Intermediate Organic Chemistry	Huigens
12	Basic & Intermediate Organic Chemistry	Huigens
<b>14</b>	<b>Exam I</b>	<b>Huigens Admin.</b>
16	Predicting Water Solubility	McCurdy
19	Ionization of Drugs (Acid/Base)	McCurdy
<b>21</b>	Ionization of Drugs (Acid/Base)	McCurdy
23	Drug/Chemical Stability	McCurdy
26	Quantitative Aspects of Drug Action	Aldrich
28	Introduction to Receptor Pharmacology	Aldrich
30	Introduction to Receptor Pharmacology – cont.	Aldrich
Oct. 3	Receptor Structure and Function: GPCRs	Aldrich
5	Receptor Structure and Function: Ligand-gated Ion Channels	Aldrich
<b>7</b>	<b>Homecoming – NO CLASS</b>	--
<b>10</b>	<b>Exam II</b>	<b>McCurdy Admin.</b>
12	Receptor Structure and Function: Receptor Tyrosine Kinases, Nuclear Receptors	Aldrich
14	Enzyme Mechanisms	Aldrich
17	Enzyme Kinetics and Inhibition	Aldrich
19	Assessing Enzyme Inhibition	Aldrich
21	Hit-to-Lead / SAR	Zheng
24	Hit-to-Lead / SAR	Zheng
26	Hit-to-Lead / SAR	Zheng
28	Hit-to-Lead / SAR	Zheng
<b>31</b>	<b>Exam III</b>	<b>Zheng Admin.</b>
Nov. 2	Introduction to Drug Absorption, Distribution & Elimination	James
4	Introduction to Pathways of Drug Metabolism	James
7	Cytochrome P450 Enzymology & Drugs that Target P450 I	James
9	Cytochrome P450 Enzymology & Drugs that target P450 II	James
11	Drugs that target P450	James
14	Importance of Stereochemistry	James
16	“Phase II” Pathways of Drug Metabolism	James
18	Reactive/Toxic Metabolites of Drugs I	James
21	Reactive/Toxic Metabolites of Drugs II	James
<b>23-25</b>	<b>Thanksgiving Break – NO CLASS</b>	--
28	Drug–Drug Interactions	Xing
30	Carcinogen Bioactivation I	Xing
Dec. 2	Carcinogen Bioactivation II	Xing
5	Conventional chemotherapeutic agents	Xing
7	Targeted anticancer therapies	Xing
<b>9</b>	<b>Exam IV</b>	<b>Xing Admin.</b>

## **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, which will involve structure, short or numerical answers. Letter grades will be assigned after each exam and final grades will be calculated with each lecture weighted equally. 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.*

### **Attendance:**

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.

### **Miscellaneous:**

#### **Students Requiring Accommodations**

Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, <https://www.dso.ufl.edu/drc>) by providing appropriate documentation. Once registered, students will receive an accommodation letter which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester.

#### **Course Evaluation**

Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at <https://evaluations.ufl.edu/evals>. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at <https://evaluations.ufl.edu/results/>.

#### **University Honesty Policy**

UF students are bound by The Honor Pledge which states, “We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: “On my honor, I have neither given nor received unauthorized aid in doing this assignment.” The Honor Code (<https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/>) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.

#### **Software Use**

All faculty, staff, and students of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

#### **Student Privacy**

There are federal laws protecting your privacy with regards to grades earned in courses and on individual assignments. For more information, please see:

<http://registrar.ufl.edu/catalog0910/policies/regulationferpa.html>

## **Campus Resources:**

### Health and Wellness

#### **U Matter, We Care:**

If you or a friend is in distress, please contact [umatter@ufl.edu](mailto:umatter@ufl.edu) or 352 392-1575 so that a team member can reach out to the student.

**Counseling and Wellness Center:** <http://www.counseling.ufl.edu/cwc>, and 392-1575; and the University Police Department: 392-1111 or 9-1-1 for emergencies.

#### **Sexual Assault Recovery Services (SARS)**

Student Health Care Center, 392-1161.

**University Police Department** at 392-1111 (or 9-1-1 for emergencies), or <http://www.police.ufl.edu/>.

### Academic Resources

**E-learning technical support**, 352-392-4357 (select option 2) or e-mail to [Learning-support@ufl.edu](mailto:Learning-support@ufl.edu).  
<https://lss.at.ufl.edu/help.shtml>.

**Career Resource Center**, Reitz Union, 392-1601. Career assistance and counseling.  
<https://www.crc.ufl.edu/>.

**Library Support**, <http://cms.uflib.ufl.edu/ask>. Various ways to receive assistance with respect to using the libraries or finding resources.

**Teaching Center**, Broward Hall, 392-2010 or 392-6420. General study skills and tutoring.  
<https://teachingcenter.ufl.edu/>.

**Writing Studio, 302 Tigert Hall**, 846-1138. Help brainstorming, formatting, and writing papers.  
<https://writing.ufl.edu/writing-studio/>.

**Student Complaints Campus:** [https://www.dso.ufl.edu/documents/UF\\_Complaints\\_policy.pdf](https://www.dso.ufl.edu/documents/UF_Complaints_policy.pdf).

**On-Line Students Complaints:** <http://www.distance.ufl.edu/student-complaint-process>.