PHA 6467C – Drug Design II

Spring 2023

Course Coordinator:
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Class Time: MWF 3:00-5:00. 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/Computational Chemistry, Analytical Chemistry, and Pharmacological Chemistry are discussed. The student will gain a general understanding of the drug design process.

Reference Text:
a. R. B. Silverman, The Organic Chemistry of Drug Design and Drug Action, 3rd Edition.
b. V. F. Roche, S. W. Zito, T. L. Lemke, and D. A. Williams, Foye's Principles of Medicinal Chemistry, 8th Edition.

Pre-requisites: Advanced undergraduate organic chemistry. Undergraduate biochemistry and Drug Design I (PHA 6447).

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 drug-target interactions, mechanism of action, pharmacophores and pharmacology of therapeutic agents.
3. Students should have a broad knowledge of the integration of different disciplines in the drug design and discovery process.
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

Date		Subject	Lecturer (Room Location)
Jan.	09	Overview of computational structure-based drug design	Li (CG-056)
	11	Molecular docking and virtual screening	Li (CG-056)
	13	Molecular dynamics simulation	Li (CG-056)
	16	**Holiday – NO CLASS**	
	18	QSAR/QSPR	Li (CG-056)
	20	Cheminformatics	Li (CG-056)
	23	AI in Drug Discovery	Li/Seabra (CG-056)
	25	Computational structure-based drug design workshop	Seabra (CG-056)
	27	Computational structure-based drug design workshop	Seabra (CG-056)
	30	Computational structure-based drug design workshop	Seabra (CG-056)
Feb.	01	Computational structure-based drug design workshop	Seabra (CG-056)
	03	Computational structure-based drug design workshop	Seabra (CG-056)
	06	Computational structure-based drug design workshop	Seabra (CG-056)
	08	Computational structure-based drug design workshop	Seabra (CG-056)
	10	**EXAM I**	CG-056
	13	Carbohydrate chemistry & Glycobiology	Cui (CG-056)
	15	Carbohydrate chemistry & Glycobiology	Cui (CG-056)
	17	Carbohydrate chemistry & Glycobiology	Cui (CG-056)
	20	Carbohydrate chemistry & Glycobiology	Cui (CG-056)
	22	Carbohydrate chemistry & Glycobiology	Cui (CG-056)
	24	CNS drugs/BBB	McCurdy (CG-056)
	27	CNS drugs Anticonvul	McCurdy (CG-056)
March	01	CNS drugs Mood	McCurdy (CG-056)
	03	CNS drugs Neurodeg	Aldrich (CG-056)
	06	CNS drugs Sub abuse	Aldrich (CG-056)
	08	CNS drugs Brain delivery	Aldrich (CG-056)
	10	**EXAM II**	CG-056
	13-17	**Spring break – NO CLASS**	
	20	Peptide drugs	Aldrich (CG-056)
	22	Natural product	Ranjala (CG-056)
	24	High-throughput screening	Ranjala (CG-056)
	27	Target identification	Ranjala (CG-056)
	29	Target identification	Ranjala (CG-056)
	31	Target identification	Ranjala (CG-056)
April	03	Antibiotics, major classes based on chemistry	Ding (CG-056)
	05	Antibiotics, MOA and resistance	Ding (CG-056)
	07	Antibiotics, MOA and resistance	Ding (CG-056)
	10	Major families of natural products and biosynthesis	Ding (CG-056)
	12	Major families of natural products and biosynthesis	Ding (CG-056)
	14	Major families of natural products and biosynthesis	Ding (CG-056)
	17	Genome-based discovery of antibiotics	Ding (CG-056)
	19	**EXAM III**	CG-056

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 **THREE** exams. They will involve structure, short or numerical answers. Students will be allowed to inspect their exams to verify their scores but exam will be kept by the faculty for three years. A letter grade will be assigned for the materials covered by each faculty. The final grade will be based on the grades of all the exams, weighed proportionally based on the number of the lectures for each exam.

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:

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.

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 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 suppor*t*, 352-392-4357 (select option 2) or e-mail to 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. **On-Line Students Complaints***: http://www.distance.ufl.edu/student-complaint-process.