Comprehensive Course Syllabus
Medicinal Chemistry

Course Description

This course will provide an in-depth look at how novel, pharmacologically active molecules are designed to treat human diseases. An overview of modern medicinal chemistry, from first principles of drug action to design and development of potential therapeutics, will be presented. The action and behavior of pharmaceutical compounds and the relationship between their structure and their chemical and therapeutic properties, and therefore, the chemical considerations in drug design will be explored. Structure activity relationships will be explored through case studies. Methods of drug discovery will be investigated, including the development of drugs from natural products, computer modeling and rational drug design.

Instructor

Instructor	Dr. John Thurmond
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Class schedule	A/C 7-8 & B/D 1-2
Office hours	AC days 11:40-12:40 or by appointment

Text(s) / Materials

No text required. Students will need a laptop computer, notebook, calculator, and pens/pencils. Students will be provided with materials such as:

- Scientific publications (J Am Board Fam Prac, JACC: Basic to translational science, BMC Medicine, Bioorganic and Medicinal Chemistry, J Med Chem, Journal of Health Economics, Nature Reviews Drug Discovery) and other medicinal chemistry topic papers.
- Software for computational medicinal chemistry (SeeSAR, molinspiration, chemsketch, PDB, admetSAR, SwissADME, pymol, autodock)

Essential Content

Students studying science at IMSA engage in the process of scientific inquiry by:

A.1 applying the skills of observation (describe, compare, and contrast characteristics; identify parameters, precisely observe phenomena) and accurately record findings. [IL-11.A.5a; IL-11.A.5c][NSES-A]
A.2 designing and planning investigations and constructing questions which further

understanding, forge connections, and deepen meaning. [IL-11.A.5b][NSES-A]
A.3 carrying out investigations that develop skills, concepts, and processes that support and enable complex thought. [IL-11.A.5c][NSES-A]
A.4 using appropriate technologies to collect, analyze and present information. [IL-11.A.5c][NSES-A]
A.5 employing scientific reasoning to evaluate the soundness and relevance of information. [IL-11.A.5e][NSES-A]
A.6 supporting judgments and constructing models based on evidence. [IL-11.A.5e][NSES-A]
A.7 sharing results by communicating orally, in writing, and through display with power, economy, and elegance. [IL-11.A.5e][NSES-A]
A.8 examining current issues in science and technology. [IL-][NSES-G]

Student Learning Objectives

Interpret the measure the activity of enzymes and receptors
Model a drug's half-life
Predict and alter the metabolism and solubility of a molecule by structural changes
Design molecules with desired biological activity for antimicrobial properties
Use various approaches including combinatorial chemistry for optimizing a molecule's structure into a safe and effective drug
Gain familiarity with the chemical nature and biochemical behavior of common classes of drug targets and modes of drug action
Understand the concepts of pharmacodynamics, pharmacokinetics, and drug metabolism and how these processes impact drug activity within the body
Be able to describe the process of drug discovery from initial compound identification and optimization

This course will require the student to integrate information, solve problems and engage in authentic inquiry to achieve these ends.

SSLs and Outcomes:
Students are expected to:
I.A Develop automaticity in skills, concepts, and processes that support and enable complex thought.

- improving lab skills
- completing homework activities and assigned readings
- design molecular compounds by applying content knowledge

I.B Construct questions which further understanding, forge connections, and deepen meaning.

- informal group discussions on drug target and molecular compound design
- apply knowledge from one drug target to another

I.C Precisely observe phenomena and accurately record findings.

- recording and analysis of laboratory data in experiments
- database of activity data and structure

I.D Evaluate the soundness and relevance of information and reasoning.

- analysis of case studies
- analysis of lab experiment data

II.A Identify unexamined cultural, historical, and personal assumptions and misconceptions that impede and skew inquiry.

- analysis of case studies
- analysis of relationship between structure and activity of molecule

III.A Use appropriate technologies as extensions of the mind.

- use of computers and software
- analysis of analytical data

III.B Recognize, pursue, and explain substantive connections within and among areas of knowledge.

- describe structure and activity relationship data
- use structural knowledge to improve ADME and toxicity properties

IV.A Construct and support judgments based on evidence.

- design novel small molecule therapeutics for various diseases
- optimize structural properties to reduce toxicity

IV.C Identify and characterize the composing elements of dynamic and organic wholes, structures, and systems.

- analysis of data from various tests to optimize beneficial properties
- use adsorption, distribution, metabolic, and excretion data to make structural changes in the molecule

V.B Make reasoned decisions which reflect ethical standards, and act in accordance with those decisions.

- present scientific data accurately

Instructional Design and Approach:

This course will provide students for a lab based course in learning the process of designing small molecules to treat human diseases. The students will be engaged in real world research using lab based experiments and computational chemistry software to optimize the beneficial properties of therapeutics. During their research, the students will explore how to bring a drug from concept to market, and how a drug's chemical structure describe the factors that affect its absorption, distribution, metabolism, and excretion, and hence the considerations to be made in drug design.

Student Expectations:

The experience you have in this course will be directly related to your level of participation. One cannot choose to be a non-participant and expect to reap all of the possible benefits. Therefore, some guidelines for a successful experience are listed below.

1. PLEASE be on time and ready for class - both mentally and physically. It is the responsibility of each student to inform the instructor and arrange for make-up work due to excused absences (preferably in advance).
   Students who are more than 5 minutes but less than 50 minutes late will be given an unexcused absence for the day. Any assignment due that day will also be considered late.

Any activity that is submitted for credit on that day can be made up by the student but will also be marked late.
Students more than 50 minutes late will also be given an unexcused absence and any assignment submitted will be marked late. NO credit will be awarded for make-up work or missed labs or activities. Refer to the Student Handbook for policies and specific effects of excessive tardies and absences.

2. Besides being on time, please have all the materials you will need for the class WITH YOU! Our classroom work on many days will require your notebook or laptop (whichever you use to take notes on), a folder for handouts, and a pen or pencil. Notebooks and/or lab data forms will be the only items allowed in the lab in which to record data. Therefore if you forget it, you cannot participate in lab work until you retrieve it!
3. Turning work in late is discouraged. When an assignment has been collected, it may be submitted for late credit at a 10% penalty per day. The student is responsible to make sure that electronic assignments are correctly submitted. Once the teacher has returned material that has been assessed, it cannot be submitted for late credit.
4. Due to the volatility of many of the organic chemicals, no personal electronic equipment may be brought into the lab. In addition, no sunglasses, food or drinks are allowed in the lab.
5. Collaboration is encouraged throughout all facets of this course. Academic dishonesty, however, is not. It is expected that students will discuss classroom activities, homework assignments and laboratory results, and partners will share common data but copying homework or lab reports is not allowed and will result in a zero on the assignment. It is also expected that all reports/work reflect individual thought and other sources will be referenced appropriately. Electronic devices cannot be used on tests or quizzes unless otherwise approved.
6. Goggles and closed-in shoes must be worn at all times in lab. A closed-in shoe covers the toes and the entire top of the foot. Keep your work/lab area neat and clean. Penalties **will** be incurred for lab areas not cleaned up. **All** IMSA materials and equipment will remain in the classroom unless given permission by the instructor. Perform only those experiments authorized by the instructor.
7. If, at any point, you are experiencing some confusion - get help ***immediately.*** Concepts cannot build upon each other if early ones are not understood. Do not wait until office hours occur. Schedule an appointment for a mutually convenient time.

Assessment Practices, Procedures, and Processes:

The grading categories and their weights:

Labs and projects (including final project) – 50%
Tests/Quizzes – 30%
Exercises – 20%

Your grade for the semester will be determined by the following standard scale:

A = 90% B = 80% C = 70%

Attendance will be mandatory in all the classes for the entire semester, consistent with IMSA policy. Students will be required to make up work on their own time.

Anticipated Topics and Activities

I. Introduction to Medicinal Chemistry, History

II. Drug Discovery Process

III. Drug Targets and Drug-Target Interactions

IV. Pharmaceutical Properties

V. Pharmacokinetics

VI. Lead Discovery and Optimization