School of pharmacy

Department Medicinal Chemistry

Course title: Practical Medicinal Chemistry
Unit: 1 unit (Practical)
***Prerequisite*:** Medicinal chemistry III
Course Lecturers: Dr. Mirfazli, Dr. Azizian, Dr. Asadi
Responsible Lecturer: Dr. Mirfazli (Saramirfazli@gmail.com)

Student responsibilities*:*

١- Preparation and presentation of determined project
٢- Collaboration is encouraged throughout all facets of this course.
٣- Tests /quizzes
٤- Midterm and final exams

واحد برنامه ریزی آموزشی دانشکده داروسازی

General Course Description

This course is designed to provide students with practical experience and basic skills in the synthesis of organic chemical compounds used as drugs or important pharmaceutical scaffolds. It also introduces the application of computational and computer-based methods in drug discovery and drug design, as well as the prediction and evaluation of the physicochemical and ADMET properties of drugs. In addition, the course covers the extraction and implementation of qualitative and quantitative pharmacopeial analytical methods, including quality-control tests, impurity testing, purity testing, and systematic qualitative analysis of chemical substances used as drugs.

General Objectives / Competency Domains

This practical course provides students with knowledge and skills related to the design, synthesis, measurement, and evaluation of drugs.

- The first section includes an introduction to commonly used software for drawing pharmaceutical structures and electronic search resources, as well as reviewing the literature to identify and evaluate methods for drug synthesis.

- The second section includes the extraction of laboratory methods for the synthesis and purification of drugs and common pharmaceutical scaffolds and their practical implementation. After synthesizing selected drugs, such as acetaminophen, benzocaine, aspirin, and coumarin scaffolds, students purify the products using various purification techniques, including recrystallization and column chromatography.
- The third section includes the assessment and evaluation of synthesized drugs using analytical methods obtained from and applicable according to pharmacopeial procedures, such as IR, UV, and HPLC, for evaluating drug purity and determining drug content, followed by comparison with pharmacopeial standards such as the USP.
- The fourth section includes developing an appropriate understanding of the physicochemical properties of drugs and how existing drugs can be developed using pharmacophore modeling, computer-based modeling techniques, and molecular docking.

Specific Objectives / Core Competencies

Upon completion of this course, students will be able to:

١. Find relevant resources and scientific articles related to the synthesis, evaluation, identification, and purification of pharmaceutical compounds and extract the required information.
٢. Perform the steps of chemical reactions for the synthesis of selected compounds according to a standard synthetic procedure.
٣. Perform appropriate purification methods for synthesized compounds.
٤. Determine the purity of synthesized compounds using conventional analytical methods, compared with reference standards, including HPLC, UV, and other appropriate techniques.
٥. Identify and apply qualitative tests for the systematic identification of unknown chemical substances.
٦. Draw and evaluate the three-dimensional structures of compounds and investigate ligand–receptor interactions using computational studies.
٧. Predict the physicochemical and ADMET properties of pharmaceutical structures based on computational studies.
٨. Develop the ability to conduct academic theses and research projects in the fields of drug design, synthesis, and preliminary evaluation within the pharmaceutical sciences.

Notes: Teachers 'classes will be held in person, students' attendance is obligatory.

Notes: All students must submit the assigned assignments (project, report, response to exercises, etc.) by the instructors on time.

Practical Medicinal Chemistry Course Schedule
Mondays: 11-13

session	Subject	Lecturer	Date
1	Introduction to and review of literature, including textbooks, electronic resources, and scientific articles, for the synthesis of Active Pharmaceutical Ingredients (APIs)	Dr. Mirfazli	**13 Mehr**
2	Training on the use of Reaxys and searching for synthetic methods	Dr. Mirfazli	**20 Mehr**
3	Principles of using and searching pharmaceutical references for the evaluation and assay of Active Pharmaceutical Ingredients (APIs)	Dr. Mirfazli	**27 Mehr**
4	Drug synthesis, Purification and identification of Acetaminophen	Dr. Asadi	**4 Aban**
5	Synthesis, Purification and identification of Benzocaine	Dr. Asadi	**11 Aban**
6	Drug assay; Assessment and evaluation of the purity of synthesized acetaminophen using HPLC and IR spectroscopy, Determination of the wavelength using a UV–Visible spectrophotometer	Dr. Mirfazli	**18 Aban**
7	Drug assay; Assessment and evaluation of the purity of synthesized Benzocaine using HPLC and IR spectroscopy, Determination of the wavelength using a UV–Visible spectrophotometer	Dr. Mirfazli	**25 Aban**
8	2D chemical structure drawing 3D representation of molecular structure	Dr. Azizian	**2 Azar**
9	In silico physico-chemical and ADMET properties prediction	Dr. Azizian	**9 Azar**
10	Minimization of molecular structure and chemical properties	Dr. Azizian	**16 Azar**
11	Investigating the Ligand-receptor interaction (1) Docking method-file preparation	Dr. Azizian	**23 Azar**
12	Investigating the Ligand-receptor interaction (2) Docking calculation and analysis	Dr. Azizian	**30 Azar**
13	Individual or group presentation of a relevant project	Dr. Azizian	**7 Day**
14	Final Exam		**14 Day**

References:

١- Pharmaceutical Substances, 5th Edition, 2009 (Syntheses, Patents and Applications of the most relevant APIs) by A. Kleemann (Author), J. Engel (Author)

٢- Reaxys (https://www.elsevier.com/products/reaxys)

٣- Vogel's Textbook of Practical Organic Chemistry (5th Edition) 5th Edition by A.I. Vogel.

٤- Organic Synthesis, Published by Organic Syntheses, Inc. ISSN 2333-3553 (online A Publication of Reliable Methods for the Preparation of Organic Compounds

٥- Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry last Edition; by Jr. Beale, John M. (Editor), John H. Block (Editor)

٦- Review of Organic Functional Groups: Introduction to Medicinal Organic Chemistry; by Zito PhD, S. William, Roche PhD, Victoria F., Lemke PhD, Thomas

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