Macao Polytechnic Institute

School of Health Sciences and Sports

Bachelor of Science in Biomedical Technology

(Pharmacy Technology)

Module Outline

Academic Year 2021 / 2022 Semester 1

Learning Module	Medicinal Chemistry			**Class Code**	BSMC2101
Pre-requisite(s)	BSOC1102 - Organic Chemistry				
Medium of Instruction	Chinese / English			**Credit**	4
Lecture Hours	36 hrs	**Lab/Practice Hours**	24 hrs	**Total Hours**	60 hrs
Instructor	Tao Yi Pedro Fong		**E-mail**	yitao@ipm.edu.mo pedrofong@ipm.edu.mo	
Office	Rm. M707 and M705, Meng Tak Building, Main Campus		**Telephone**	8599 3471 (Tao Yi) 8599 3427 (Pedro)	

Description

This learning module describes the basic principles of medicinal chemistry. Key concepts in drug discovery, lead compound identification & development, combinatorial chemistry, chiral drugs, structure-activity relationship (SAR), quantitative structure-activity relationship (QSAR), and computer-aided drug design will be introduced. The teaching format is based on lectures, tutorials, case studies, laboratory practicals and computer modelling sessions.

Learning Outcomes

After completing the learning module, students will be able to:

1. Describe the key concepts of medicinal chemistry
2. Apply the key concepts of medicinal chemistry into pharmacy practice
3. Apply the principles of interactions between small molecules and biological macromolecules to predict binding affinity
4. Perform common molecular modelling techniques
5. Predict ADMET from the structure of drugs

Content

1. Overview of medicinal chemistry (22 hours)

1.1 Introduction

Students will be able to describe the key concepts of medicinal chemistry, including lead compound, analogue, SAR, QSAR, pharmacophore, drug-likeness, Lipinski's rules and high-throughput screening.

1.2 Drug structure and solubility

Students will be able to infer solubility from the structure of drugs and illustrate general methods of changing drug solubility.

1.3 Drug targets

Students will be able to describe structures and functions of receptors and enzymes, distinguish between different types of receptors and enzymes, analyze the relationship between drug structure and target affinity, and illustrate general methods of design of agonists and antagonists.

1.4 Stability of drugs and Kinetics of drug stability

Students will be able to describe degradation pathways of pharmaceuticals and accelerated stability test methods, measure influences of pH and temperature on degradation, and calculate shelf-life by Arrhenius law.

2. Drug discovery (2 hours)

2.1 Students will be able to understand and perform some basic drug discovery processes based on the following topics:

2.1.1 Choosing a disease
2.1.2 Choosing a drug target
2.1.3 Identifying a bioassay
2.1.4 Finding a lead compound
2.1.5 Isolation and purification
2.1.6 Structure determination

3. Drug design (4 hours)

3.1 Students will be able to understand and perform some basic drug design processes based on the following topics:

3.1.1 Optimizing target interactions
3.1.2 Structure-activity relationships
3.1.3 Identification of a pharmacophore
3.1.4 Strategies in drug optimization
3.1.5 Optimizing access to the target
3.1.6 Resistant to chemical and enzymatic degradation

3.1.7 Resistant to drug metabolism
3.1.8 Reducing toxicity
3.1.9 Prodrugs

4. Getting the drug to market (2 hours)
   4.1 Students will be able to understand the fundamental processes of getting a new drug to market:
   4.1.1 Preclinical and clinical trials
   4.1.2 Patenting and regulatory affairs
   4.1.3 Chemical and process development
   4.1.4 Case studies: The design of ACE inhibitors, artemisinin and related antimalarial drugs and the design of oxamniquine

5. Computers in medicinal chemistry (4 hours)
   5.1 Students will be able to describe and perform basic techniques on computational chemistry:
   5.1.1 Molecular and quantum mechanics
   5.1.2 Molecular dimensions and properties
   5.1.3 Energy minimization
   5.1.4 Docking procedures – manual, automatic, rigid and flexible docking
   5.1.5 Automated screening of database for lead compounds
   5.1.6 Quantitative structure-activity relationship

6. Presentation (2 hours)

Class Practice (Dr Yi Tao, 8 hours)

Date & Time	Practice Item	Title	Students / Group	Mode of Practice	Requirement
2021/10/07 14:30-18:30	Preparation & characterization of aspirin by chemical synthesis in laboratory scale	Drug obtained from chemical synthesis	Grouping	Operating in the laboratory	Each group should complete the experiment and submit the experiment report.
2021/10/21 14:30-18:30	Accelerated stability test, content determination by UV spectrophotometry	Stability of ascorbic acid under accelerated conditions	Grouping	Operating in the laboratory	Each group should complete the experiment and submit the experiment report.

Class Practice (Dr Pedro Fong, 16 hours)

Date & Time	Practice Item	Title	Students / Group	Mode of Practice	Requirement
2021/08/30 14:30-16:30 AND 2021/08/31 14:30-16:30	Preparation of structures for computational modelling I	Generate 2D and 3D molecular structures	Individual	Computational	Each student should complete all the required tasks.
2021/09/06 14:30-16:30 AND 2021/09/07 14:30-16:30	Preparation of structures for computational modelling II	Protein structural preparation and energy minimisation	Individual	Computational	Each student should complete all the required tasks.
2021/09/13 14:30-16:30 AND 2021/08/31 14:30-16:30	Perform computational modelling I	Identify lead compounds by screening database	Individual	Computational	Each student should complete all the required tasks.
2021/09/14 14:30-16:30 AND 2021/09/20 14:30-16:30	Perform computational modelling II	ADMET prediction	Individual	Computational	Each student should complete all the required tasks.

Teaching Method

Lectures, videos, case studies, group discussion

Attendance

Attendance requirements are governed by the "Academic Regulations Governing Bachelor's Degree Programmes of Macao Polytechnic Institute". An "F" will be given as the final grade to students who have less than the stated attendance for the enrolled learning module.

Assessment

This learning module is graded on a 100 point scale, with 100 being the highest possible score and 50 being the passing score.

	Item	Description	Percentage
1.	Practical 1 (Aaron)	Laboratory report	5%
2.	Practical 2 (Aaron)	Laboratory report	5%
3.	Group discussion (Aaron)	Topic will be announced in class	5%
5.	In-class exercises (Aaron)	Overview of medicinal chemistry	35%
6.	Presentation (Pedro)	Topic will be announced in class	15%
7.	Assignment (Pedro)	Small scale research report	35%
		Total Percentage:	100%

Any student attaining less than 90% in practical sessions will be given an "F' grade, regardless of the score achieved in the course works and assignment.

Teaching Material(s)

Textbook(s)

Graham Patrick. (2018) An Introduction to Medicinal Chemistry (Sixth Edition). Oxford University Press, UK.

Reference

Reference book(s)

M. E. Aulton. (2021) Aulton's Pharmaceutics: The Design and Manufacture of Medicines (6th edition). Elsevier, U.K.

N. Brown. (2016) In Silico Medicinal Chemistry: Computational Methods to Support Drug Design. Royal Society of Chemistry, UK.

G. Thomas. (2007) Medicinal Chemistry. John Wiley & Sons Ltd, England.