澳門理工大學
Universidade Politécnica de Macau
Macao Polytechnic University

FACULTY OF APPLIED SCIENCES

DOCTOR OF PHILOSOPHY IN ARTIFICIAL INTELLIGENCE DRIVEN DRUG DISCOVERY

LEARNING MODULE OUTLINE

Academic Year	2024/2025	Semester	1
Module Code	AIDD8124		
Learning Module	Chemobioinformatics		
Pre-requisite(s)	None		
Medium of Instruction	Chinese and English		
Credits	3	Contact Hours	45
Instructor	Zhang Qianqian Li Kefeng Wei Leyi	Email	zhangqq@mpu.edu.mo
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MODULE DESCRIPTION

Chemobioinformatics is a field of study that bridges two important areas of pharmaceutical sciences: chemoinformatics and bioinformatics. Despite their historical separation, these areas are now more interconnected than ever before. This course provides an introduction to chemobioinformatics and its applications to drugs, omics, chemical biology, protein function, and biomedicine. Topics covered include databases, omics analysis, proteins, and their interactions, chemical descriptions of proteins and organic compounds, data modeling, QSAR modelling, proteochemometrics modelling, drug discovery and development, and the use of chemobioinformatics software.

MODULE INTENDED LEARNING OUTCOMES (ILOS)

On completion of this learning module, students will be able to:

M1.	Apply a comprehensive knowledge of how chemobioinformatics tools can be used in drug discovery and the basic theories of omic analysis, computational methods in drug design, including structure-based and ligand-based drug design. (AHEP4-M1, AHEP4-M3)
M2.	Critically evaluate and select proper computational strategies and be able to use them to solve the practical drug design and discovery problems. (AHEP4-M2, AHEP4-M4)
M3.	Select and apply appropriate chemobioinformatics tools and drug design software, such as MOE, omics techniques to perform target identification, network pharmacology analysis, molecular docking, virtual screening, de novo drug design, QSAR and pharmacophore model. (AHEP4-M1, AHEP4-M3)
M4.	Work in a team for a complete an advanced drug discovery research topic, design and evaluate solutions for a real-world problem, and finally present it in class. (AHEP4-M4, AHEP4-M5, AHEP4-M6, AHEP4-M16, AHEP4-M17)

These ILOs aims to enable students to attain the following Programme Intended Learning Outcomes (PILOs):

PILOs	M1	M2	M3	M4
P1. Understand the databases and retrieval methods related to small molecules and proteins	✓	✓		
P2. Understand the basic concept of computational methods in drug discovery and development	✓	✓		
P3. Master the virtual screening method based on molecular docking and pharmacophore model	✓	✓	✓	
P4. Master the drawing skills of drug design related software	✓	✓	✓	
P5. Understand the structure of medical data	✓			✓
P6. Understanding how omic techniques are utilized in identifying the drug targets	✓			✓
P7. Become proficient in the application of open-source large omics datasets using AI techniques	✓			✓

MODULE SCHEDULE, COVERAGE AND STUDY LOAD

Week	Content Coverage	Contact Hours
1	1. Introduction to drug discovery and development	3
	1.1 History of drug Discovery	
	1.2 The modern drug discovery and development process	
	1.3 Introduction to computer-aided drug design	
	1.4 Introduction to artificial intelligence drug design	
2-3	2. Introduction to drug target types and protein structure prediction	6
	2.1 The basic concept of drug target	
	2.2 Receptor as drug target	
	2.3 Enzyme as drug target	
	2.4 Protein structure and function	
	2.5 Protein structure prediction using computer	
4-5	3. Introduction to structure-based drug discovery	6
	3.1 Molecular docking	
	3.2 Scoring function	
	3.3 Docking Program	
	3.4 De novo drug design	

6-8	4.	Introduction to ligand-based drug discovery	9
	4.1	Conformational Sampling of Ligand	
	4.2	Fingerprint/Descriptors-based search	
	4.3	Pharmacophore model	
	4.4	Quantitative structure–activity relationships (QSAR) model	
9-10	5.	Deep learning-based molecule generation	6
	5.1	Molecular Representation	
	5.2	Databases and Benchmark Datasets	
	5.3	Machine Learning Tools	
	5.4	Evaluation metrics	
11-15	6.	Introduction to modern biology and bioinformatics	15
	6.1	Overview and techniques of genomics	
	6.2	Overview and techniques of transcriptomics	
	6.3	Overview and techniques of proteomics	
	6.4	Overview and techniques of metabolomics and exposomics	

TEACHING AND LEARNING ACTIVITIES

In this learning module, students will work towards attaining the ILOs through the following teaching and learning activities:

Teaching and Learning Activities	**M1**	**M2**	**M3**	**M4**
T1. Lectures	✓		✓	
T2. In-class exercises		✓		✓

ATTENDANCE

Attendance requirements are governed by the Academic Regulations Governing Doctoral's Degree Programmes of the Macao Polytechnic University. Students who do not meet the attendance requirements for the learning module shall be awarded an 'F' grade.

ASSESSMENT

In this learning module, students are required to complete the following assessment activities:

Assessment Activities	**Weighting (%)**	**AHEP4 LOs**	**ILOs to be Assessed**
A1. Course work (Dr. Zhang)	25	AHEP4-M1, AHEP4-M2,	M1, M2, M3

		AHEP4-M3, AHEP4-M4	
A2. Assignment (Dr. Li)	25	AHEP4-M1, AHEP4-M2, AHEP4-M3, AHEP4-M4,	M1, M2, M3
A3. Project (Dr. Zhang)	50	AHEP4-M4,AHEP4-M5, AHEP4-M6, AHEP4-M16, AHEP4-M17	M1, M2, M3, M4

The assessment will be conducted following the University's Assessment Strategy (see www.mpu.edu.mo/teaching_learning/en/assessment_strategy.php). Passing this learning module indicates that students will have attained the ILOs of this learning module and thus acquired its credits.

MARKING SCHEME

NA

REQUIRED READINGS

There are no official required readings for this module. Module notes are distributed in the class.

REFERENCES

1. Wikberg at al., 2020, Introduction to Pharmaceutical Bioinformatics, Oakleaf Academic.

2.Navneet Sharma, et al., 2021, Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences, Elsevier Inc.

3.Jeffrey J-P Tsai, Ka-Lok Ng, 2019. Application of Omics, AI, and Blockchain in Bioinformatics Research. World Scientific Publisher.

STUDENT FEEDBACK

At the end of every semester, students are invited to provide feedback on the learning module and the teaching arrangement through questionnaires. Your feedback is valuable for instructors to enhance the module and its delivery for future students. The instructor and programme coordinators will consider all feedback and respond with actions formally in the annual programme review.

ACADEMIC INTEGRITY

The Macao Polytechnic University requires students to have full commitment to academic integrity when engaging in research and academic activities. Violations of academic integrity, which include but are not limited to plagiarism, collusion, fabrication or falsification, repeated use of assignments and cheating in examinations, are considered as serious academic offenses and may lead to disciplinary actions. Students should read the relevant regulations and guidelines in the Student Handbook which is distributed upon the admission into the University, a copy of which can also be found at www.mpu.edu.mo/student_handbook/.